Full wwPDB NMR Structure Validation Report (i)

Jun 6, 2023 – 01:54 pm BST

PDB ID	:	5JZR
BMRB ID	:	30094
Title	:	Solid-state MAS NMR structure of Acinetobacter phage 205 (AP205) coat protein in assembled capsid particles
Authors	:	Jaudzems, K.; Andreas, L.B.; Stanek, J.; Lalli, D.; Bertarello, A.; Le Marchand, T.; Cala-De Paepe, D.; Kotelovica, S.; Akopjana, I.; Knott, B.; Wegner, S.; Engelke, F.; Lesage, A.; Emsley, L.; Tars, K.; Herrmann, T.; Pintacuda, G.
Deposited on	:	2016-05-17

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

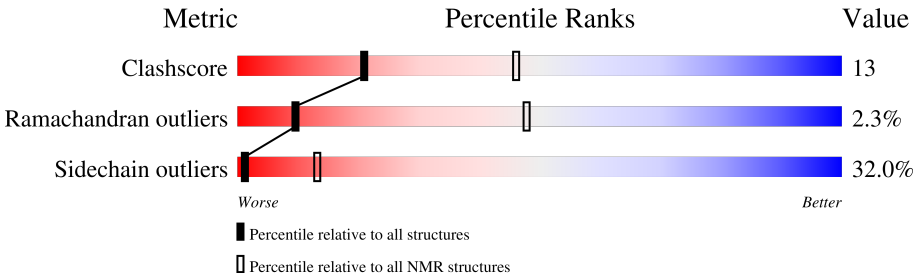
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
SOLID-STATE NMR

The overall completeness of chemical shifts assignment is 35%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	131	41% 34% · 24%
1	B	131	41% 34% · 24%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 7 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:4-A:8, A:15-A:35, A:44-A:59, A:72-A:128, B:204-B:208, B:215-B:235, B:244-B:259, B:272-B:328 (198)	1.60	7

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 4 clusters and 2 single-model clusters were found.

Cluster number	Models
1	10, 13, 14, 15, 18, 20
2	1, 7, 8, 11, 16
3	2, 3, 12, 19
4	4, 5, 6
Single-model clusters	9; 17

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 3936 atoms, of which 1974 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Coat protein.

Mol	Chain	Residues	Atoms						Trace
1	A	131	Total	C	H	N	O	S	0
			1968	610	987	173	193	5	
1	B	131	Total	C	H	N	O	S	0
			1968	610	987	173	193	5	

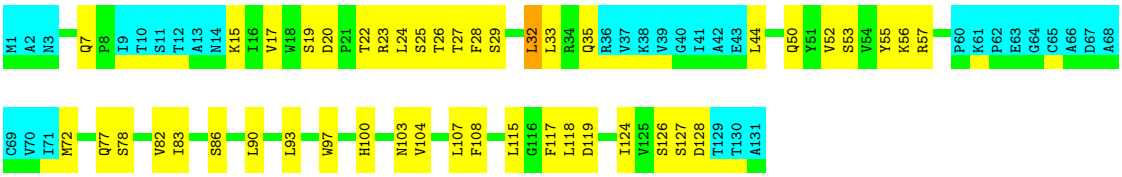
4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

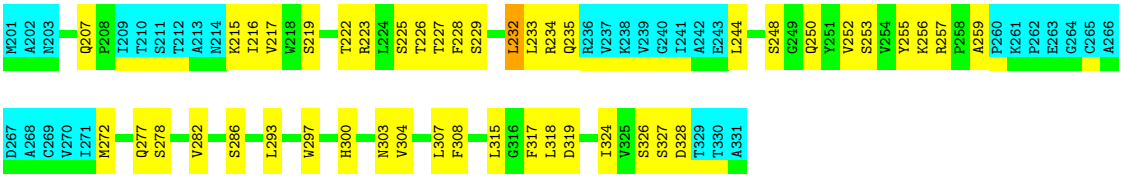
• Molecule 1: Coat protein

Chain A:



• Molecule 1: Coat protein

Chain B:



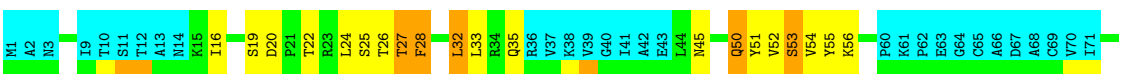
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

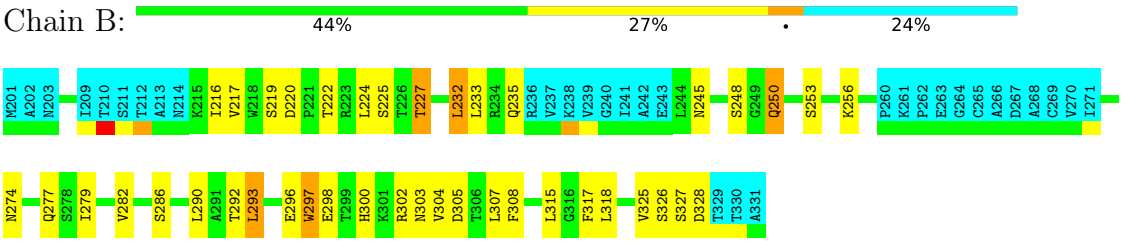
4.2.1 Score per residue for model 1

• Molecule 1: Coat protein

Chain A:

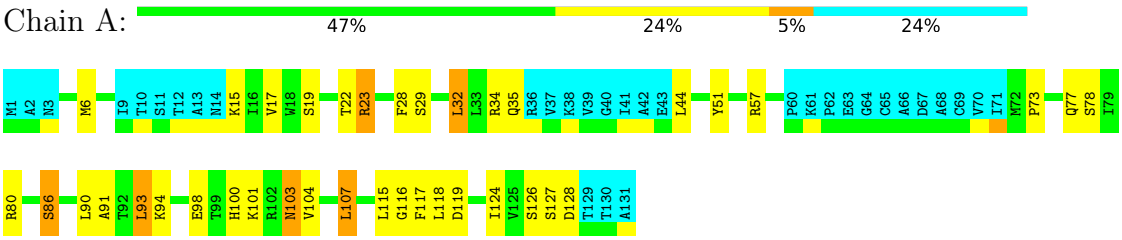


• Molecule 1: Coat protein

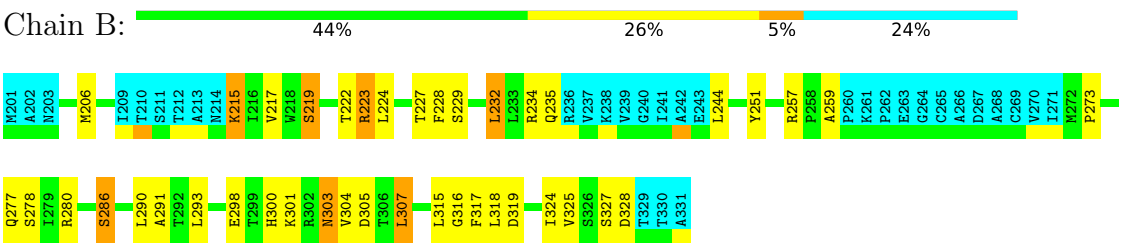


4.2.2 Score per residue for model 2

• Molecule 1: Coat protein

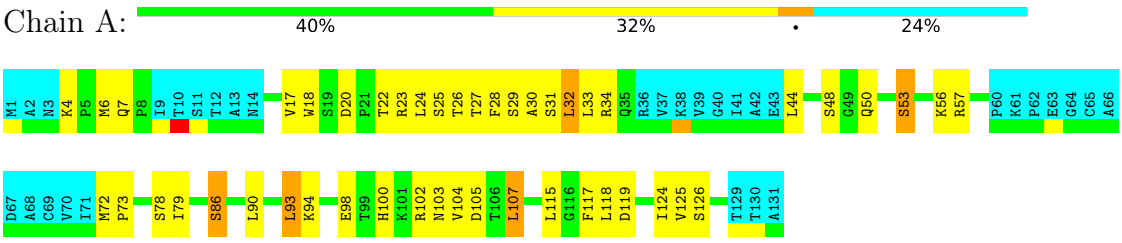


• Molecule 1: Coat protein



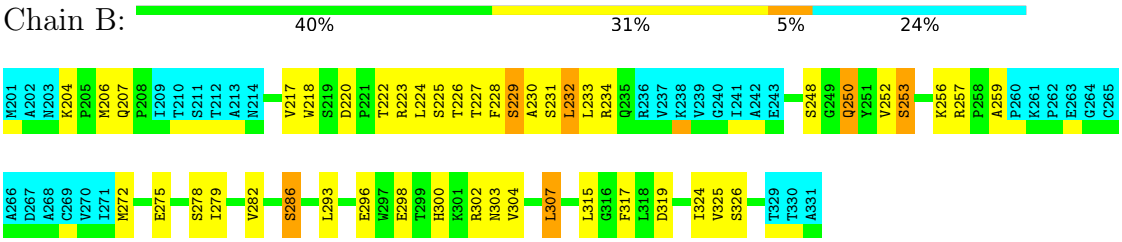
4.2.3 Score per residue for model 3

• Molecule 1: Coat protein



• Molecule 1: Coat protein

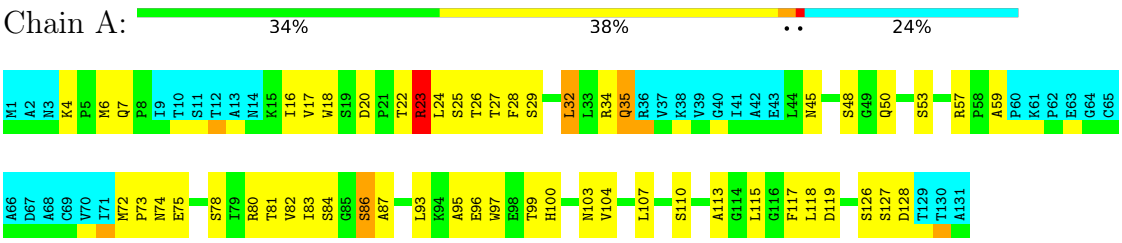
Chain B:



4.2.4 Score per residue for model 4

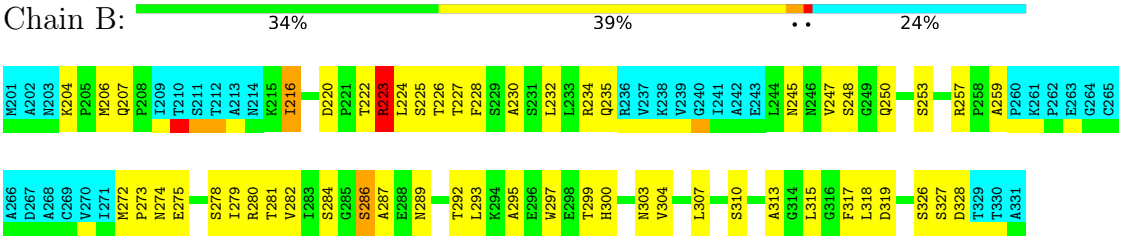
• Molecule 1: Coat protein

Chain A:



• Molecule 1: Coat protein

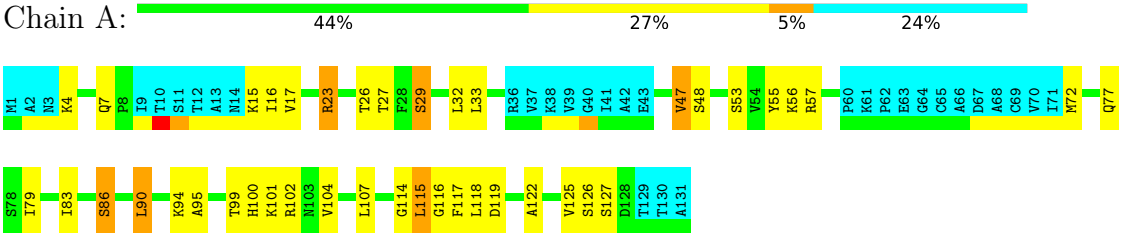
Chain B:



4.2.5 Score per residue for model 5

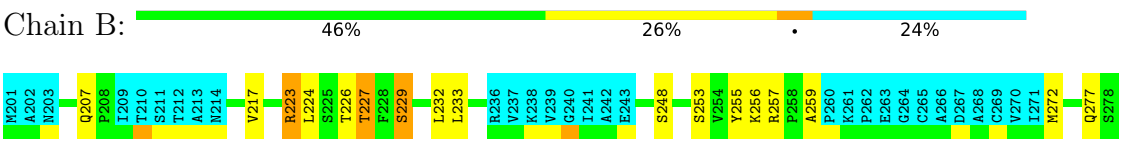
• Molecule 1: Coat protein

Chain A:



• Molecule 1: Coat protein

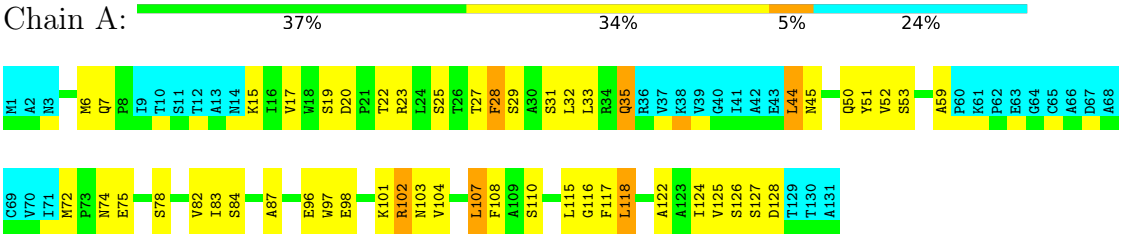
Chain B:



4.2.6 Score per residue for model 6

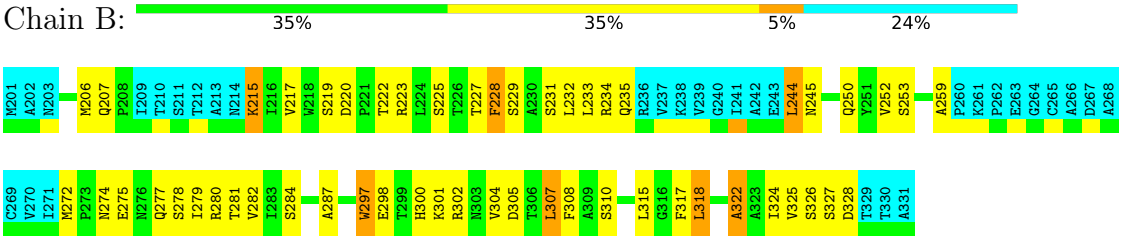
• Molecule 1: Coat protein

Chain A:



• Molecule 1: Coat protein

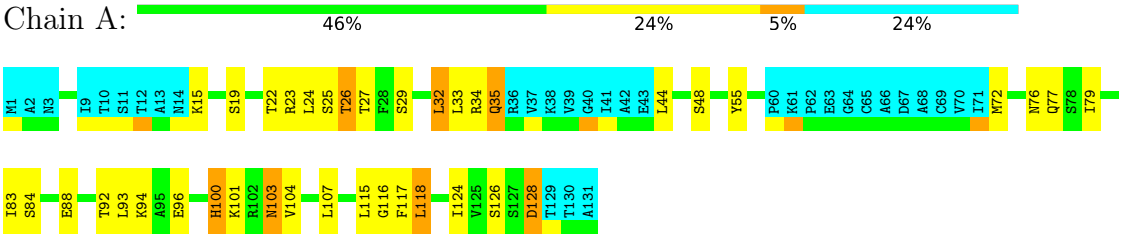
Chain B:



4.2.7 Score per residue for model 7 (medoid)

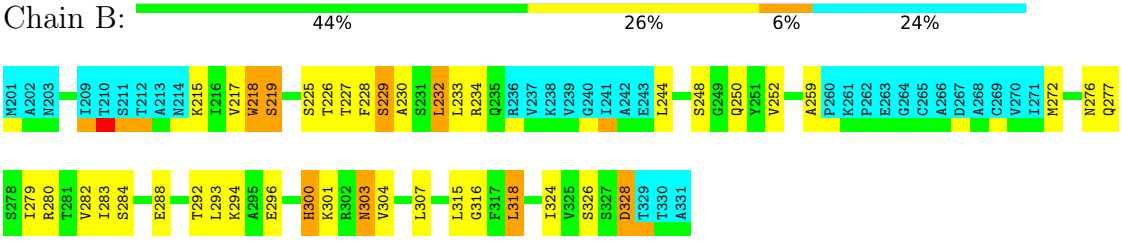
• Molecule 1: Coat protein

Chain A:



• Molecule 1: Coat protein

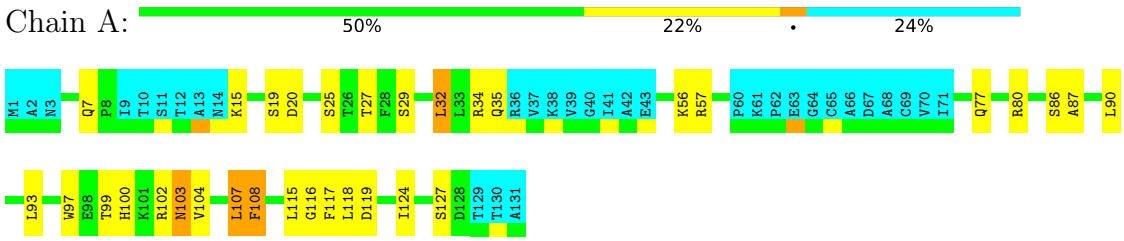
Chain B:



4.2.8 Score per residue for model 8

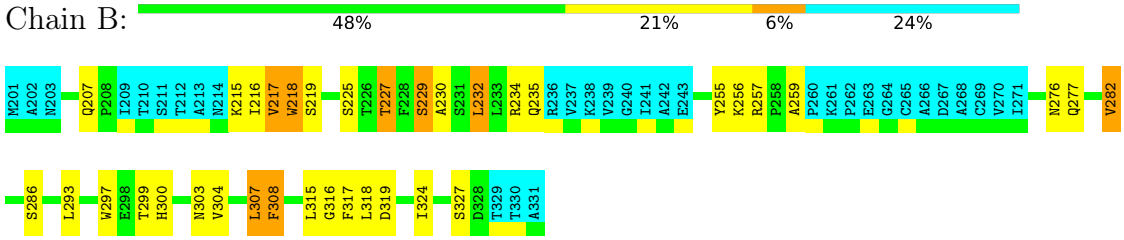
• Molecule 1: Coat protein

Chain A:



• Molecule 1: Coat protein

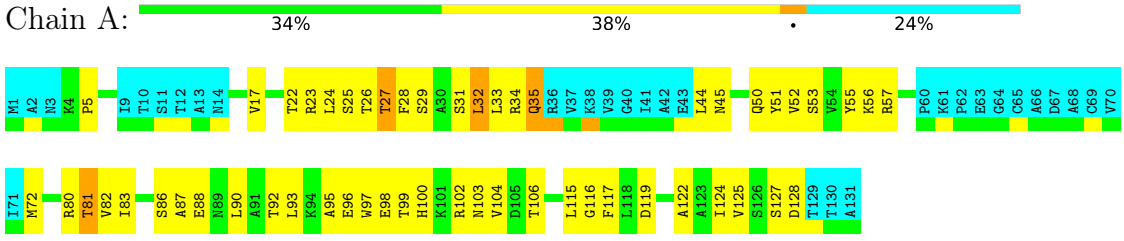
Chain B:



4.2.9 Score per residue for model 9

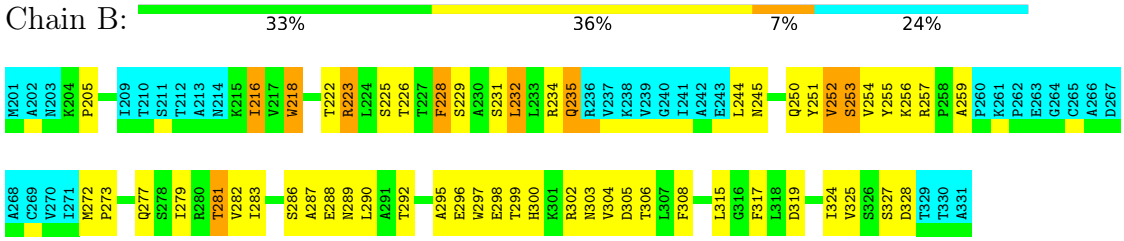
• Molecule 1: Coat protein

Chain A:



• Molecule 1: Coat protein

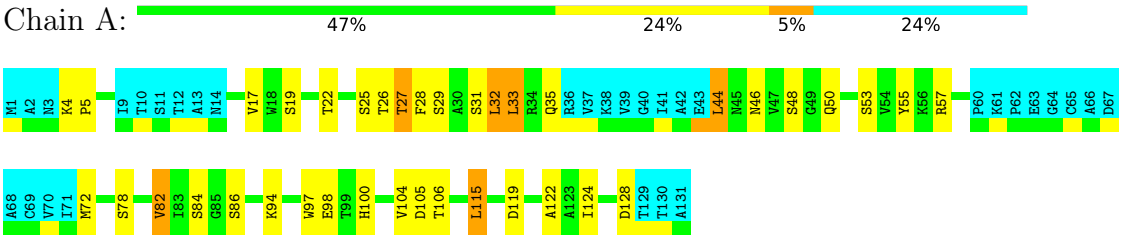
Chain B:



4.2.10 Score per residue for model 10

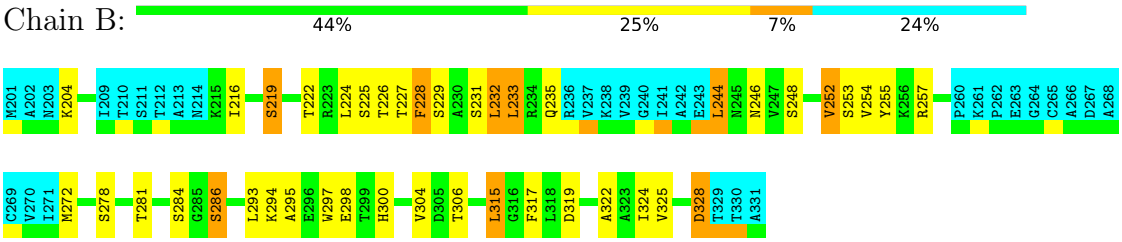
• Molecule 1: Coat protein

Chain A:



• Molecule 1: Coat protein

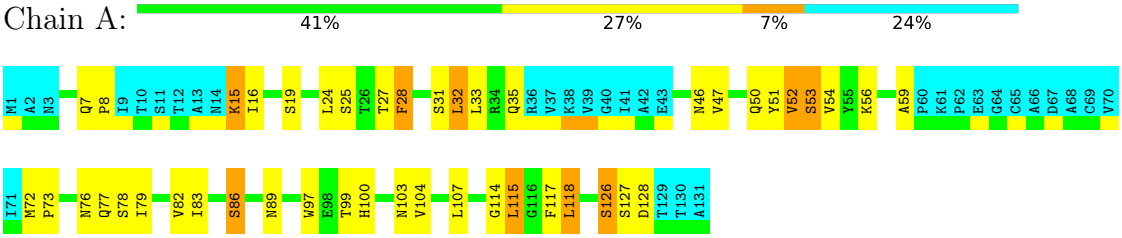
Chain B:



4.2.11 Score per residue for model 11

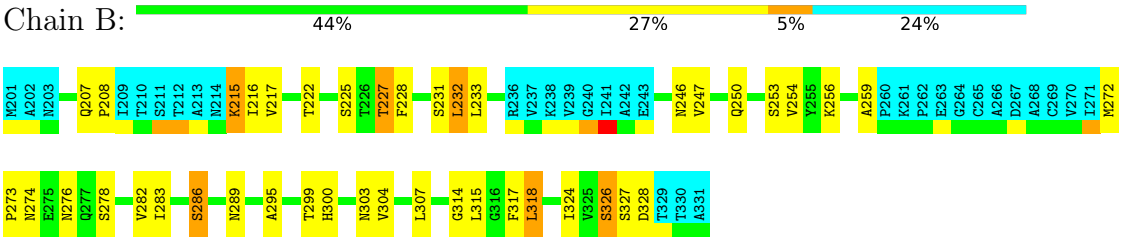
• Molecule 1: Coat protein

Chain A:



• Molecule 1: Coat protein

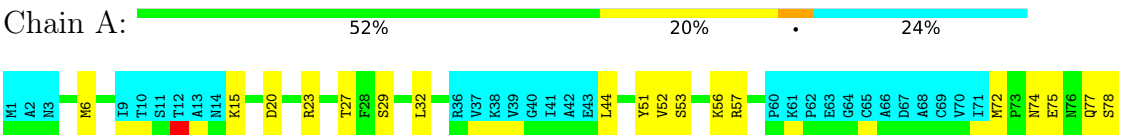
Chain B:

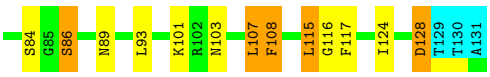


4.2.12 Score per residue for model 12

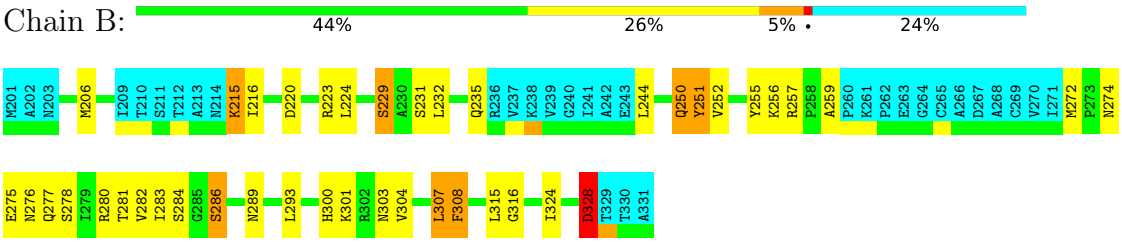
• Molecule 1: Coat protein

Chain A:



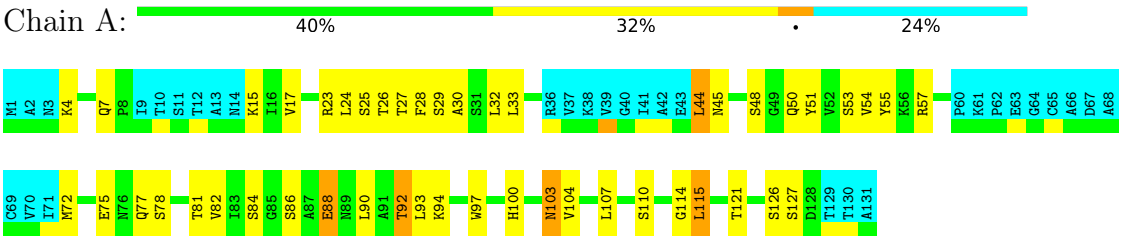


• Molecule 1: Coat protein

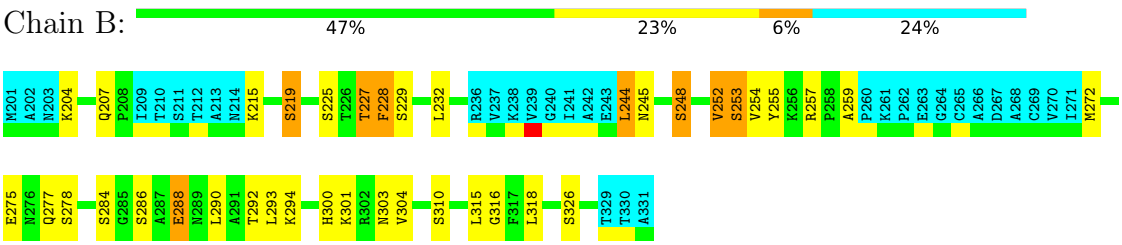


4.2.13 Score per residue for model 13

• Molecule 1: Coat protein

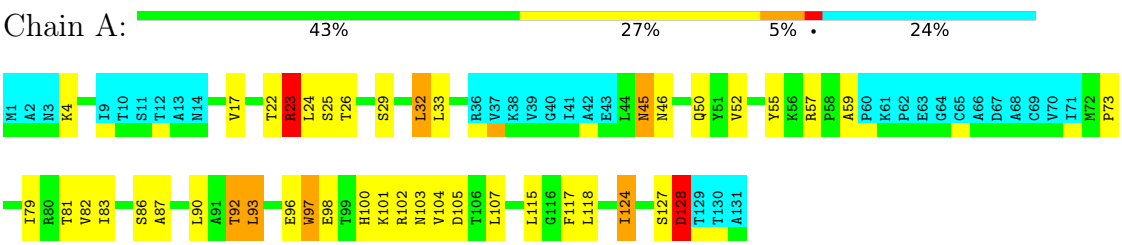


• Molecule 1: Coat protein

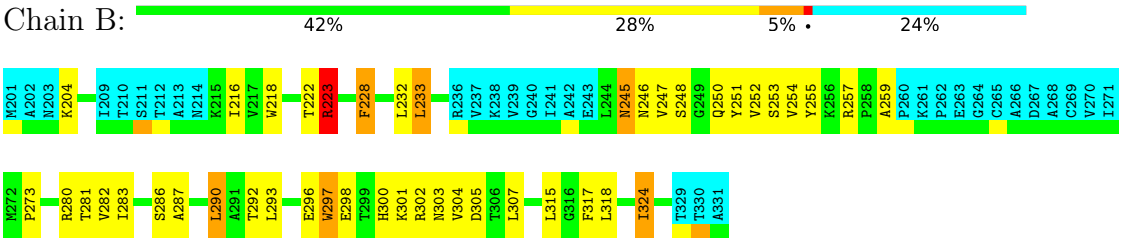


4.2.14 Score per residue for model 14

• Molecule 1: Coat protein

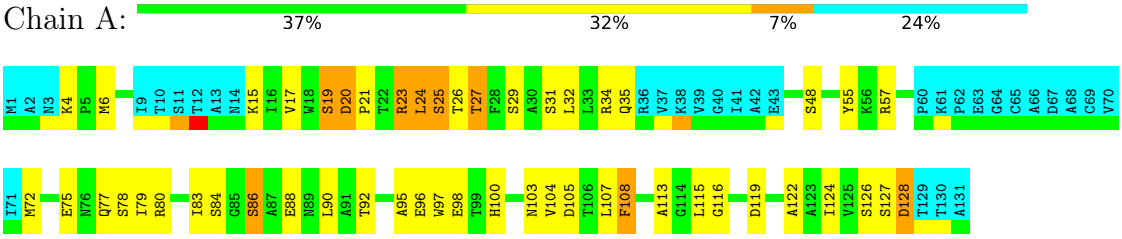


• Molecule 1: Coat protein

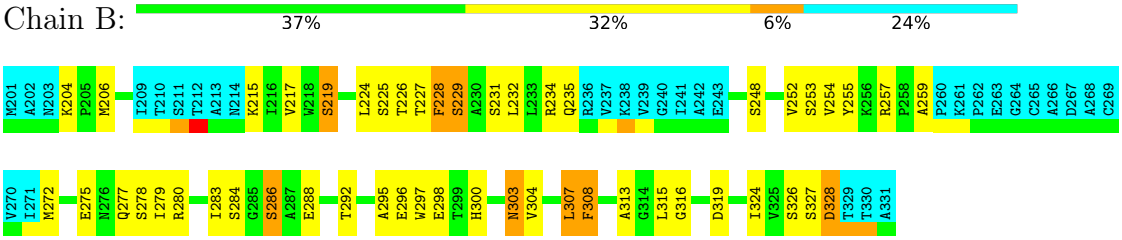


4.2.15 Score per residue for model 15

• Molecule 1: Coat protein

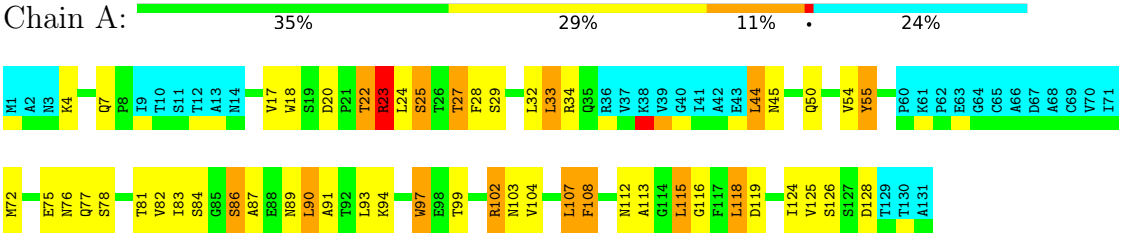


• Molecule 1: Coat protein

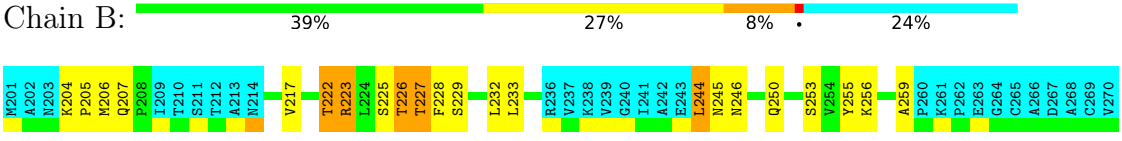


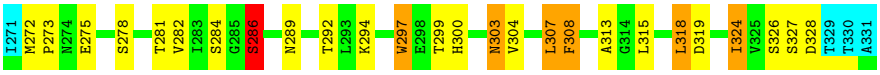
4.2.16 Score per residue for model 16

• Molecule 1: Coat protein



• Molecule 1: Coat protein

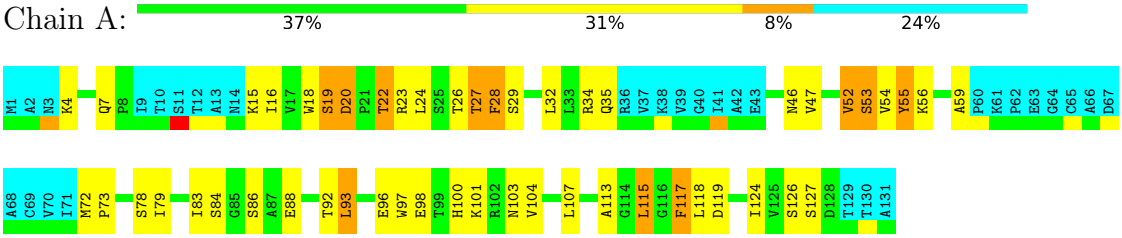




4.2.17 Score per residue for model 17

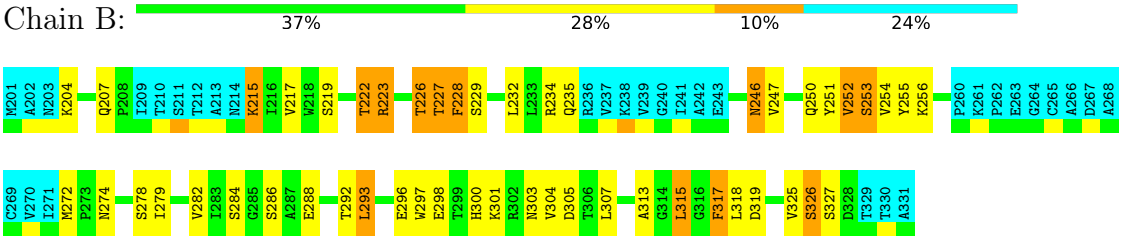
• Molecule 1: Coat protein

Chain A:



• Molecule 1: Coat protein

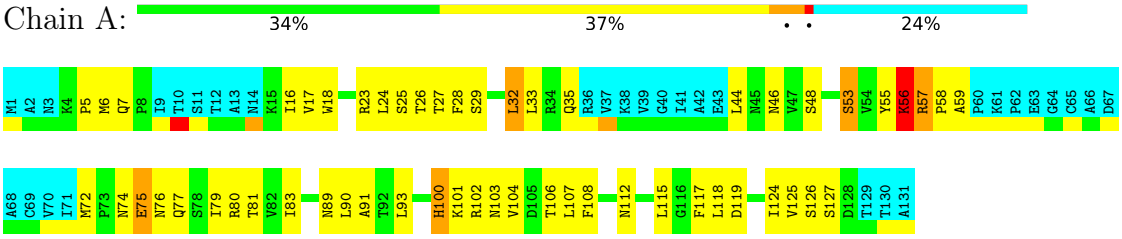
Chain B:



4.2.18 Score per residue for model 18

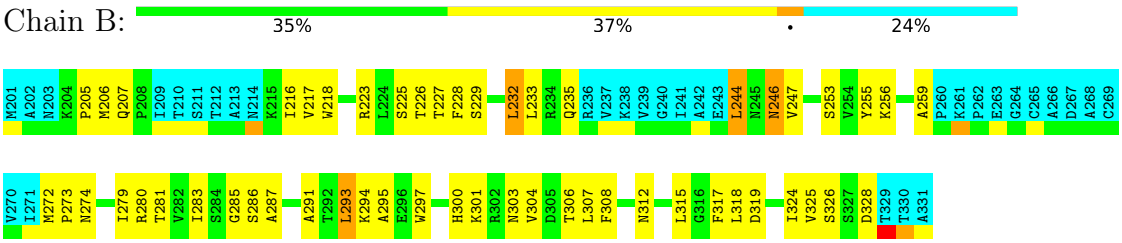
• Molecule 1: Coat protein

Chain A:



• Molecule 1: Coat protein

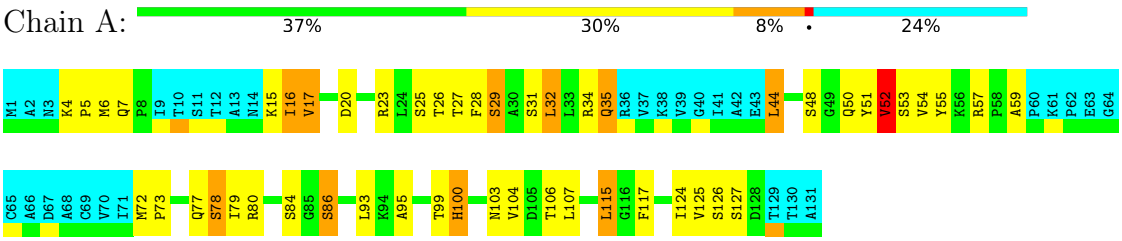
Chain B:



4.2.19 Score per residue for model 19

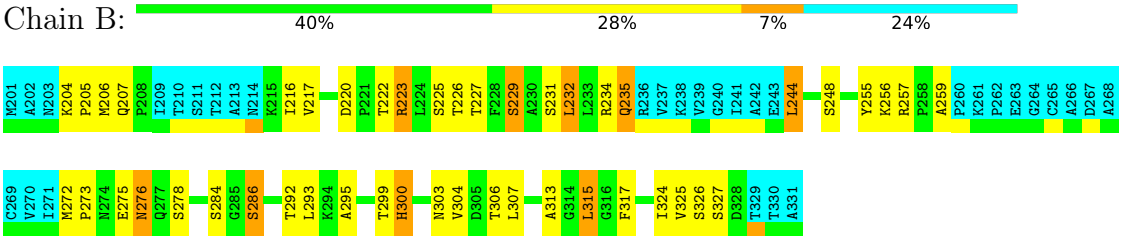
• Molecule 1: Coat protein

Chain A:



• Molecule 1: Coat protein

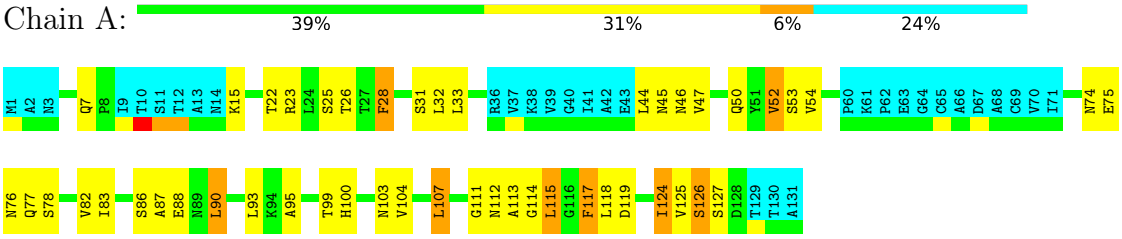
Chain B:



4.2.20 Score per residue for model 20

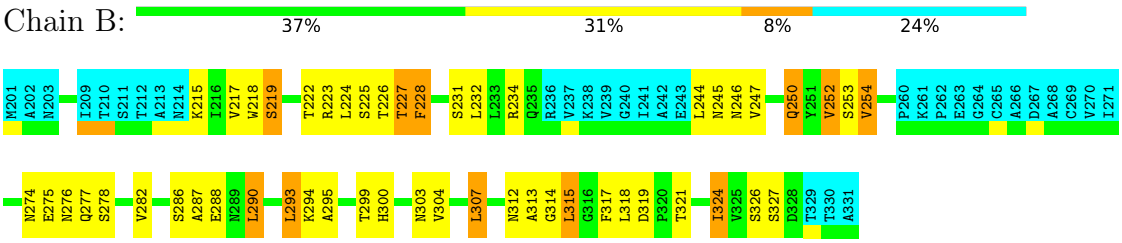
• Molecule 1: Coat protein

Chain A:



• Molecule 1: Coat protein

Chain B:



5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
UNIO	structure calculation	2.6
CYANA	structure calculation	3.97

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1021
Number of shifts mapped to atoms	1021
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	35%

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

6 Model quality

6.1 Standard geometry

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	759	758	758	24±8
1	B	759	758	758	23±6
All	All	30360	30320	30320	807

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:107:LEU:HD11	1:A:118:LEU:HD22	0.92	1.41	6	1
1:B:228:PHE:CD1	1:B:254:VAL:HG23	0.91	2.01	15	4
1:B:307:LEU:HD11	1:B:318:LEU:HD22	0.91	1.43	6	1
1:A:24:LEU:HD11	1:B:299:THR:HG21	0.90	1.38	4	1
1:B:228:PHE:CD2	1:B:254:VAL:HG23	0.87	2.05	13	2
1:A:90:LEU:HD13	1:A:91:ALA:N	0.86	1.86	1	1
1:B:217:VAL:HG21	1:B:227:THR:HG22	0.83	1.49	11	1
1:A:28:PHE:CD1	1:A:54:VAL:HG23	0.80	2.11	11	2
1:A:90:LEU:C	1:A:90:LEU:HD22	0.80	1.96	1	1
1:A:28:PHE:CD2	1:A:54:VAL:HG23	0.80	2.10	17	1
1:A:27:THR:O	1:A:54:VAL:HG12	0.80	1.76	1	1
1:A:99:THR:HG21	1:B:224:LEU:HD11	0.78	1.55	4	1
1:B:244:LEU:HD12	1:B:287:ALA:HB3	0.78	1.54	18	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:52:VAL:HG21	1:A:80:ARG:HA	0.77	1.55	19	1
1:B:250:GLN:CB	1:B:282:VAL:HA	0.77	2.09	12	1
1:A:95:ALA:O	1:A:99:THR:HG23	0.76	1.81	4	5
1:A:83:ILE:HG21	1:A:93:LEU:HD12	0.76	1.57	16	1
1:A:32:LEU:HD22	1:A:32:LEU:C	0.75	2.02	11	7
1:A:26:THR:HG21	1:A:55:TYR:CD2	0.75	2.17	14	2
1:B:227:THR:O	1:B:254:VAL:HG12	0.75	1.82	20	1
1:B:232:LEU:C	1:B:232:LEU:HD22	0.75	2.02	11	5
1:B:217:VAL:HG22	1:B:227:THR:HG22	0.74	1.59	16	2
1:B:228:PHE:HB3	1:B:252:VAL:O	0.74	1.83	14	7
1:A:90:LEU:HD23	1:A:91:ALA:N	0.73	1.99	16	1
1:A:113:ALA:HB1	1:B:247:VAL:HG13	0.72	1.60	20	1
1:A:28:PHE:CB	1:A:53:SER:HA	0.72	2.14	1	5
1:B:217:VAL:CG2	1:B:227:THR:HG22	0.72	2.12	11	3
1:A:28:PHE:HB3	1:A:52:VAL:O	0.72	1.83	20	4
1:B:252:VAL:HG12	1:B:280:ARG:HA	0.72	1.60	14	3
1:A:107:LEU:HD13	1:A:118:LEU:HD11	0.72	1.60	20	1
1:A:97:TRP:CZ2	1:B:304:VAL:HG11	0.71	2.20	6	4
1:B:255:TYR:O	1:B:276:ASN:HB3	0.71	1.86	19	1
1:A:47:VAL:HG21	1:A:90:LEU:HD23	0.70	1.64	20	1
1:A:47:VAL:HG13	1:B:313:ALA:HB1	0.70	1.63	20	1
1:A:87:ALA:O	1:A:90:LEU:HD12	0.69	1.88	1	1
1:B:228:PHE:CG	1:B:252:VAL:HG13	0.69	2.22	15	1
1:B:295:ALA:O	1:B:299:THR:HG23	0.69	1.87	4	5
1:B:226:THR:HG22	1:B:255:TYR:CD1	0.69	2.22	16	1
1:A:107:LEU:HD12	1:B:232:LEU:HD23	0.68	1.64	20	1
1:B:229:SER:O	1:B:251:TYR:HB3	0.68	1.87	12	1
1:B:219:SER:HB3	1:B:227:THR:HG23	0.67	1.67	13	2
1:A:90:LEU:HD13	1:A:91:ALA:H	0.67	1.49	1	1
1:A:26:THR:HG21	1:A:55:TYR:CD1	0.67	2.24	13	2
1:A:108:PHE:CZ	1:A:113:ALA:HB3	0.66	2.25	16	2
1:B:250:GLN:HB2	1:B:282:VAL:HG22	0.65	1.68	16	2
1:A:28:PHE:CE1	1:A:54:VAL:HG23	0.65	2.26	11	1
1:A:100:HIS:O	1:A:104:VAL:HG23	0.65	1.91	11	15
1:A:107:LEU:HD11	1:A:118:LEU:HD12	0.65	1.68	2	1
1:B:315:LEU:HD12	1:B:317:PHE:HB2	0.65	1.68	17	2
1:B:247:VAL:HG21	1:B:290:LEU:HD23	0.64	1.66	20	1
1:A:104:VAL:HG11	1:B:297:TRP:CZ2	0.64	2.26	6	5
1:A:116:GLY:CA	1:B:232:LEU:HD11	0.64	2.23	15	2
1:A:103:ASN:HA	1:A:124:ILE:HD12	0.64	1.70	2	4
1:A:57:ARG:HB2	1:A:58:PRO:HD2	0.64	1.67	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:217:VAL:HG23	1:B:228:PHE:C	0.64	2.13	18	5
1:A:115:LEU:HD12	1:A:117:PHE:HB2	0.64	1.69	17	2
1:A:96:GLU:OE2	1:B:279:ILE:HD11	0.63	1.93	17	2
1:A:116:GLY:HA3	1:B:232:LEU:HD13	0.63	1.71	16	2
1:A:79:ILE:HG23	1:B:283:ILE:HG13	0.63	1.68	14	3
1:A:32:LEU:HD11	1:B:316:GLY:CA	0.63	2.24	12	2
1:A:99:THR:HG22	1:A:127:SER:CB	0.63	2.23	8	1
1:B:299:THR:HG23	1:B:326:SER:HA	0.63	1.71	16	2
1:A:92:THR:HG21	1:B:255:TYR:CE2	0.63	2.28	9	1
1:B:300:HIS:O	1:B:304:VAL:HG23	0.63	1.94	11	16
1:A:32:LEU:HD22	1:A:33:LEU:N	0.62	2.09	10	6
1:B:259:ALA:HB3	1:B:273:PRO:O	0.62	1.94	18	2
1:B:259:ALA:HB3	1:B:273:PRO:HG2	0.62	1.71	2	4
1:B:303:ASN:HA	1:B:324:ILE:HD12	0.62	1.71	8	5
1:B:245:ASN:CB	1:B:287:ALA:HB2	0.62	2.25	6	2
1:B:302:ARG:HD3	1:B:325:VAL:HG23	0.62	1.70	6	2
1:A:52:VAL:HB	1:A:79:ILE:O	0.62	1.95	19	1
1:A:50:GLN:HB2	1:A:82:VAL:HG22	0.62	1.70	4	1
1:A:17:VAL:HG12	1:A:29:SER:CB	0.61	2.25	4	2
1:A:114:GLY:C	1:A:115:LEU:HD13	0.61	2.16	13	4
1:A:45:ASN:CB	1:A:87:ALA:HB2	0.61	2.25	6	2
1:A:117:PHE:O	1:A:118:LEU:HD22	0.61	1.94	20	2
1:B:307:LEU:HD21	1:B:318:LEU:HD21	0.61	1.73	16	1
1:A:17:VAL:HG23	1:A:28:PHE:C	0.61	2.16	6	5
1:A:17:VAL:HG12	1:A:29:SER:HB2	0.61	1.73	14	1
1:B:303:ASN:O	1:B:324:ILE:HD11	0.60	1.96	16	4
1:A:83:ILE:CG1	1:B:279:ILE:HG23	0.60	2.27	7	1
1:A:55:TYR:HA	1:A:77:GLN:O	0.60	1.96	16	1
1:A:102:ARG:CD	1:A:125:VAL:HG23	0.60	2.26	5	1
1:A:48:SER:O	1:B:313:ALA:HB1	0.60	1.96	4	1
1:B:314:GLY:C	1:B:315:LEU:HD13	0.60	2.17	5	2
1:A:20:ASP:CB	1:A:23:ARG:HD2	0.60	2.27	15	1
1:B:299:THR:HG22	1:B:327:SER:HB3	0.60	1.73	8	1
1:B:232:LEU:HD22	1:B:233:LEU:N	0.60	2.10	1	4
1:B:293:LEU:O	1:B:293:LEU:HD22	0.60	1.97	20	2
1:B:283:ILE:HG21	1:B:293:LEU:CD2	0.59	2.27	14	1
1:B:228:PHE:CD1	1:B:252:VAL:HG22	0.59	2.32	15	1
1:B:228:PHE:CG	1:B:252:VAL:HG23	0.59	2.32	14	1
1:A:116:GLY:HA2	1:B:232:LEU:HD11	0.59	1.73	15	2
1:B:250:GLN:OE1	1:B:281:THR:HG23	0.59	1.98	12	1
1:B:217:VAL:HG12	1:B:229:SER:HB2	0.59	1.73	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:90:LEU:HD22	1:A:90:LEU:O	0.59	1.96	1	1
1:A:107:LEU:HD23	1:A:124:ILE:HD11	0.59	1.75	12	2
1:A:118:LEU:HD12	1:A:122:ALA:HB2	0.59	1.73	6	1
1:A:52:VAL:HG11	1:A:80:ARG:CA	0.59	2.28	19	1
1:B:302:ARG:CD	1:B:325:VAL:HG23	0.59	2.27	5	1
1:A:92:THR:HG22	1:A:96:GLU:HG3	0.59	1.73	9	4
1:B:250:GLN:HB3	1:B:281:THR:O	0.59	1.98	12	1
1:A:17:VAL:HG12	1:A:27:THR:HG22	0.59	1.73	10	2
1:A:23:ARG:HG2	1:A:24:LEU:N	0.58	2.12	15	1
1:A:44:LEU:HD21	1:A:86:SER:CB	0.58	2.28	19	1
1:A:108:PHE:CE1	1:B:293:LEU:HD22	0.58	2.33	12	1
1:A:26:THR:HG22	1:A:55:TYR:CD2	0.58	2.32	10	2
1:A:93:LEU:HD22	1:A:93:LEU:O	0.58	1.98	3	2
1:A:45:ASN:HB2	1:A:87:ALA:HB2	0.58	1.76	6	1
1:A:113:ALA:HB1	1:B:248:SER:O	0.58	1.98	4	1
1:A:32:LEU:HD11	1:B:316:GLY:HA2	0.58	1.74	15	2
1:A:5:PRO:HA	1:B:325:VAL:HG12	0.57	1.76	19	4
1:B:245:ASN:HB2	1:B:287:ALA:HB2	0.57	1.75	6	1
1:B:232:LEU:HD22	1:B:232:LEU:O	0.57	1.99	19	2
1:A:32:LEU:HD22	1:A:32:LEU:O	0.57	2.00	19	2
1:B:307:LEU:HD11	1:B:318:LEU:HD12	0.57	1.75	2	1
1:B:219:SER:CB	1:B:227:THR:HG23	0.57	2.30	13	4
1:A:75:GLU:CG	1:B:244:LEU:HD21	0.57	2.30	12	1
1:A:26:THR:HG22	1:A:55:TYR:HA	0.57	1.76	1	1
1:A:83:ILE:HG23	1:B:279:ILE:HG12	0.57	1.75	18	5
1:A:81:THR:HG23	1:B:281:THR:HG23	0.57	1.77	9	1
1:A:17:VAL:HG22	1:A:27:THR:CG2	0.57	2.29	16	1
1:A:116:GLY:HA2	1:B:232:LEU:HD13	0.57	1.76	5	3
1:A:52:VAL:HG13	1:A:80:ARG:HG2	0.57	1.76	9	1
1:A:55:TYR:HB3	1:A:77:GLN:C	0.57	2.20	16	1
1:A:103:ASN:O	1:A:124:ILE:HD11	0.57	2.00	20	3
1:A:107:LEU:HD12	1:B:232:LEU:CD2	0.57	2.30	20	1
1:A:17:VAL:CG2	1:A:27:THR:HG22	0.56	2.30	9	1
1:B:315:LEU:HD12	1:B:317:PHE:CB	0.56	2.30	10	2
1:A:55:TYR:CB	1:A:77:GLN:N	0.56	2.68	16	1
1:B:303:ASN:CA	1:B:324:ILE:HD11	0.56	2.31	14	4
1:B:217:VAL:HG22	1:B:227:THR:CG2	0.56	2.29	16	2
1:A:125:VAL:HG12	1:B:205:PRO:HA	0.56	1.76	19	4
1:B:277:GLN:NE2	1:B:279:ILE:HD11	0.56	2.16	9	1
1:A:95:ALA:HB1	1:A:128:ASP:O	0.56	2.01	15	1
1:B:226:THR:HG22	1:B:255:TYR:HB2	0.56	1.78	18	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:56:LYS:O	1:A:76:ASN:HA	0.56	2.01	18	1
1:B:295:ALA:HB1	1:B:328:ASP:O	0.56	2.00	10	2
1:A:32:LEU:HD13	1:B:316:GLY:HA2	0.56	1.75	5	3
1:B:218:TRP:HA	1:B:218:TRP:CE3	0.56	2.35	7	2
1:B:232:LEU:HD12	1:B:233:LEU:N	0.56	2.16	14	1
1:B:219:SER:OG	1:B:227:THR:HG23	0.56	2.00	15	1
1:A:28:PHE:HB2	1:A:53:SER:HA	0.55	1.77	1	1
1:A:93:LEU:HD22	1:B:308:PHE:CZ	0.55	2.36	9	1
1:B:302:ARG:CG	1:B:325:VAL:HG23	0.55	2.32	3	1
1:A:19:SER:HB3	1:A:27:THR:HG23	0.55	1.78	17	2
1:B:219:SER:OG	1:B:227:THR:HG22	0.55	2.02	2	1
1:B:226:THR:HG22	1:B:255:TYR:CD2	0.55	2.36	5	1
1:A:99:THR:HG22	1:A:127:SER:HB2	0.55	1.77	8	1
1:B:289:ASN:HA	1:B:292:THR:HG22	0.55	1.78	4	2
1:A:83:ILE:CG2	1:A:93:LEU:HD12	0.55	2.30	16	1
1:A:108:PHE:CZ	1:B:293:LEU:HD12	0.55	2.37	8	1
1:A:23:ARG:CG	1:A:24:LEU:N	0.55	2.70	15	2
1:B:303:ASN:OD1	1:B:304:VAL:HG23	0.55	2.02	1	1
1:A:79:ILE:HD11	1:B:296:GLU:CD	0.55	2.21	17	2
1:A:103:ASN:CA	1:A:124:ILE:HD11	0.55	2.31	14	3
1:A:83:ILE:HG13	1:B:279:ILE:HG23	0.55	1.77	7	1
1:A:93:LEU:HD12	1:B:308:PHE:CZ	0.55	2.36	8	1
1:A:116:GLY:HA2	1:B:232:LEU:HD21	0.55	1.79	9	1
1:B:228:PHE:CE2	1:B:254:VAL:HG23	0.55	2.37	9	2
1:B:232:LEU:HD13	1:B:248:SER:O	0.55	2.02	14	1
1:A:90:LEU:HD23	1:A:91:ALA:H	0.55	1.61	16	1
1:B:232:LEU:HD12	1:B:248:SER:O	0.54	2.02	13	1
1:A:50:GLN:HG3	1:A:82:VAL:HG22	0.54	1.79	6	3
1:B:292:THR:HG22	1:B:296:GLU:HG3	0.54	1.79	1	4
1:B:307:LEU:CD2	1:B:324:ILE:HD11	0.54	2.32	12	2
1:A:17:VAL:CG1	1:A:27:THR:HG22	0.54	2.32	10	1
1:B:228:PHE:CE1	1:B:254:VAL:HG23	0.54	2.37	15	4
1:A:115:LEU:HD22	1:A:115:LEU:N	0.54	2.18	20	4
1:A:107:LEU:HD11	1:A:118:LEU:CD2	0.54	2.33	16	2
1:B:228:PHE:CB	1:B:253:SER:HA	0.54	2.32	15	7
1:B:232:LEU:C	1:B:232:LEU:CD2	0.54	2.75	11	4
1:A:79:ILE:HG23	1:B:283:ILE:CG1	0.54	2.33	14	3
1:A:19:SER:OG	1:A:27:THR:HG23	0.54	2.02	15	1
1:B:217:VAL:HG13	1:B:217:VAL:O	0.54	2.01	16	2
1:A:15:LYS:HB3	1:A:16:ILE:HD12	0.54	1.79	11	1
1:A:96:GLU:CD	1:B:279:ILE:HD11	0.54	2.23	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:83:ILE:HG12	1:B:279:ILE:HG23	0.53	1.80	5	1
1:A:102:ARG:NH1	1:A:125:VAL:HG23	0.53	2.18	6	1
1:A:107:LEU:HD21	1:A:118:LEU:CD2	0.53	2.34	16	1
1:B:246:ASN:HB3	1:B:285:GLY:O	0.53	2.03	18	1
1:A:44:LEU:HD21	1:B:275:GLU:CG	0.53	2.34	12	1
1:B:293:LEU:HD13	1:B:294:LYS:N	0.53	2.18	20	2
1:A:106:THR:HB	1:A:124:ILE:HD13	0.53	1.79	19	4
1:A:16:ILE:HD12	1:A:18:TRP:CZ2	0.53	2.38	18	1
1:B:250:GLN:CG	1:B:282:VAL:HG22	0.53	2.33	11	4
1:B:256:LYS:C	1:B:276:ASN:OD1	0.53	2.47	19	1
1:A:93:LEU:HD22	1:B:308:PHE:CE1	0.53	2.38	12	2
1:A:32:LEU:HD22	1:B:316:GLY:CA	0.53	2.34	2	1
1:A:102:ARG:HD3	1:A:125:VAL:HG23	0.53	1.80	5	1
1:A:32:LEU:C	1:A:32:LEU:CD2	0.53	2.75	1	7
1:B:315:LEU:HD12	1:B:317:PHE:HB3	0.53	1.79	10	1
1:A:32:LEU:HD23	1:B:307:LEU:HD12	0.53	1.81	15	1
1:B:228:PHE:CE1	1:B:252:VAL:HG22	0.53	2.38	15	1
1:A:44:LEU:HD13	1:B:275:GLU:HG3	0.52	1.81	6	1
1:A:75:GLU:CG	1:B:244:LEU:HD13	0.52	2.34	6	1
1:A:107:LEU:CD1	1:A:118:LEU:HD21	0.52	2.35	20	1
1:A:44:LEU:HD21	1:B:275:GLU:HG2	0.52	1.79	3	1
1:A:32:LEU:HD22	1:B:316:GLY:HA3	0.52	1.81	5	1
1:A:115:LEU:HD12	1:A:117:PHE:CB	0.52	2.34	17	1
1:A:51:TYR:C	1:A:52:VAL:HG22	0.52	2.25	19	1
1:B:216:ILE:O	1:B:229:SER:HA	0.52	2.05	8	2
1:A:26:THR:HG22	1:A:55:TYR:CD1	0.52	2.40	7	3
1:B:232:LEU:C	1:B:232:LEU:HD13	0.52	2.24	1	1
1:B:290:LEU:HD12	1:B:290:LEU:O	0.52	2.04	1	1
1:A:55:TYR:CA	1:A:77:GLN:O	0.52	2.56	16	1
1:A:102:ARG:CG	1:A:125:VAL:HG23	0.52	2.35	3	1
1:A:117:PHE:C	1:A:118:LEU:HD23	0.52	2.24	7	1
1:A:103:ASN:OD1	1:A:104:VAL:HG23	0.52	2.05	1	1
1:B:250:GLN:HG3	1:B:282:VAL:HG22	0.52	1.81	4	2
1:A:44:LEU:HD13	1:B:275:GLU:CG	0.52	2.34	6	1
1:A:28:PHE:HA	1:A:53:SER:CB	0.52	2.35	19	1
1:A:50:GLN:HB2	1:A:82:VAL:HG23	0.52	1.81	9	2
1:A:17:VAL:HG22	1:A:27:THR:HG22	0.52	1.82	16	1
1:A:44:LEU:HD23	1:A:87:ALA:HB3	0.52	1.81	9	1
1:A:32:LEU:C	1:A:32:LEU:HD13	0.52	2.25	10	1
1:A:44:LEU:HD21	1:A:88:GLU:OE2	0.52	2.05	7	1
1:B:306:THR:HB	1:B:324:ILE:HD13	0.52	1.79	19	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:229:SER:O	1:B:252:VAL:HG12	0.52	2.04	15	1
1:A:59:ALA:HB3	1:A:73:PRO:O	0.52	2.04	19	1
1:A:107:LEU:CD1	1:A:118:LEU:HD22	0.51	2.28	6	1
1:A:115:LEU:HD13	1:A:117:PHE:CD1	0.51	2.40	12	1
1:A:92:THR:HG21	1:B:255:TYR:CD1	0.51	2.40	13	1
1:B:317:PHE:O	1:B:318:LEU:HD22	0.51	2.04	11	1
1:A:28:PHE:CZ	1:A:30:ALA:HB2	0.51	2.39	13	1
1:A:19:SER:HB2	1:A:27:THR:HG23	0.51	1.82	1	1
1:B:303:ASN:HA	1:B:324:ILE:HD11	0.51	1.81	14	3
1:A:23:ARG:HD3	1:A:24:LEU:H	0.51	1.65	15	1
1:A:55:TYR:HB2	1:A:77:GLN:CB	0.51	2.35	18	1
1:A:44:LEU:HD21	1:B:275:GLU:OE1	0.51	2.06	20	1
1:B:307:LEU:HD23	1:B:324:ILE:HD11	0.51	1.83	12	2
1:A:44:LEU:HD23	1:A:86:SER:CB	0.51	2.36	10	2
1:B:224:LEU:HB3	1:B:226:THR:HG22	0.51	1.82	4	1
1:A:5:PRO:CA	1:B:325:VAL:HG12	0.51	2.36	9	2
1:A:28:PHE:HB3	1:A:53:SER:HA	0.51	1.83	17	3
1:A:99:THR:HG23	1:A:126:SER:HA	0.51	1.82	16	2
1:B:217:VAL:HG13	1:B:228:PHE:C	0.51	2.27	3	1
1:B:315:LEU:HD22	1:B:315:LEU:N	0.51	2.20	5	2
1:A:20:ASP:CB	1:A:21:PRO:HD2	0.51	2.36	15	1
1:B:250:GLN:HB2	1:B:282:VAL:HG23	0.50	1.83	6	4
1:A:107:LEU:CD2	1:A:124:ILE:HD11	0.50	2.36	2	2
1:A:125:VAL:HG12	1:B:205:PRO:CA	0.50	2.36	9	1
1:A:20:ASP:H	1:A:23:ARG:NE	0.50	2.04	15	1
1:A:24:LEU:HB3	1:A:26:THR:HG22	0.50	1.81	4	1
1:B:308:PHE:CZ	1:B:313:ALA:HB3	0.50	2.41	15	2
1:B:255:TYR:O	1:B:276:ASN:CB	0.50	2.56	19	1
1:A:79:ILE:HG21	1:B:300:HIS:CD2	0.50	2.42	17	1
1:A:32:LEU:HD13	1:A:32:LEU:O	0.50	2.06	10	1
1:A:87:ALA:O	1:A:90:LEU:HD22	0.50	2.07	16	1
1:B:244:LEU:HD11	1:B:286:SER:HB2	0.50	1.83	19	1
1:A:107:LEU:HD23	1:A:124:ILE:HD13	0.50	1.83	20	1
1:A:28:PHE:CD2	1:A:53:SER:HB3	0.50	2.42	19	1
1:B:217:VAL:HG13	1:B:228:PHE:CA	0.50	2.37	20	1
1:B:244:LEU:HD23	1:B:286:SER:HB3	0.50	1.84	10	2
1:A:75:GLU:HG3	1:B:244:LEU:HD13	0.49	1.82	6	1
1:A:100:HIS:C	1:A:100:HIS:CD2	0.49	2.86	1	1
1:B:300:HIS:CD2	1:B:300:HIS:C	0.49	2.86	1	1
1:B:232:LEU:HD12	1:B:233:LEU:H	0.49	1.67	14	1
1:A:79:ILE:HG12	1:B:283:ILE:HG23	0.49	1.84	14	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:307:LEU:HD11	1:B:318:LEU:HD23	0.49	1.85	16	1
1:A:75:GLU:OE1	1:B:244:LEU:HD21	0.49	2.07	20	1
1:A:103:ASN:O	1:A:107:LEU:HD23	0.49	2.07	11	2
1:A:44:LEU:HD21	1:A:86:SER:HB3	0.49	1.83	19	1
1:A:56:LYS:C	1:A:75:GLU:O	0.49	2.50	18	1
1:B:244:LEU:CD1	1:B:287:ALA:HB3	0.49	2.32	18	2
1:B:293:LEU:HD22	1:B:293:LEU:C	0.49	2.28	18	2
1:B:226:THR:HG21	1:B:255:TYR:CZ	0.49	2.43	10	2
1:B:310:SER:O	1:B:318:LEU:HD13	0.49	2.06	13	1
1:A:107:LEU:HD21	1:A:118:LEU:HD21	0.49	1.83	16	1
1:A:50:GLN:CG	1:A:82:VAL:HG22	0.49	2.37	14	4
1:B:232:LEU:HD13	1:B:232:LEU:O	0.49	2.08	1	1
1:A:59:ALA:HB3	1:A:73:PRO:HG2	0.49	1.85	17	3
1:A:24:LEU:HD22	1:A:55:TYR:CE1	0.49	2.43	13	1
1:A:20:ASP:CB	1:A:23:ARG:HB3	0.49	2.37	15	1
1:B:307:LEU:HD11	1:B:318:LEU:CD2	0.49	2.38	16	1
1:A:116:GLY:HA3	1:B:232:LEU:HD22	0.49	1.84	2	3
1:A:52:VAL:CB	1:A:79:ILE:O	0.49	2.60	19	1
1:A:103:ASN:HA	1:A:124:ILE:HD11	0.48	1.85	14	2
1:A:23:ARG:H	1:A:23:ARG:CD	0.48	2.21	15	1
1:B:293:LEU:HD12	1:B:297:TRP:CE3	0.48	2.43	1	1
1:A:32:LEU:HD11	1:B:316:GLY:HA3	0.48	1.84	13	1
1:B:228:PHE:HB2	1:B:253:SER:HA	0.48	1.84	20	2
1:A:81:THR:HG23	1:B:281:THR:OG1	0.48	2.06	18	1
1:A:93:LEU:HD13	1:A:94:LYS:N	0.48	2.23	2	2
1:B:226:THR:HG22	1:B:255:TYR:CG	0.48	2.43	5	1
1:A:32:LEU:O	1:A:32:LEU:HD13	0.48	2.08	14	2
1:B:229:SER:OG	1:B:252:VAL:HG12	0.48	2.09	7	1
1:A:44:LEU:HD23	1:A:86:SER:HB3	0.48	1.86	10	2
1:B:217:VAL:HA	1:B:228:PHE:O	0.48	2.07	11	2
1:B:244:LEU:HD23	1:B:286:SER:CB	0.48	2.38	10	2
1:A:50:GLN:O	1:A:51:TYR:CD1	0.48	2.67	19	1
1:A:116:GLY:CA	1:B:232:LEU:HD13	0.48	2.38	6	1
1:B:247:VAL:HG21	1:B:290:LEU:CD2	0.48	2.38	14	1
1:B:228:PHE:CE1	1:B:252:VAL:CG2	0.48	2.97	15	1
1:B:302:ARG:HG3	1:B:325:VAL:HG23	0.48	1.86	3	1
1:B:224:LEU:HD22	1:B:255:TYR:OH	0.48	2.08	12	1
1:B:216:ILE:HD12	1:B:218:TRP:CZ2	0.48	2.44	18	1
1:B:318:LEU:HD12	1:B:322:ALA:HB2	0.48	1.84	6	1
1:B:318:LEU:HD13	1:B:319:ASP:N	0.48	2.24	16	1
1:A:26:THR:HG22	1:A:55:TYR:CG	0.48	2.44	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:217:VAL:HG23	1:B:228:PHE:N	0.48	2.24	17	1
1:A:24:LEU:CB	1:A:26:THR:HG23	0.47	2.39	7	1
1:B:246:ASN:CB	1:B:286:SER:HA	0.47	2.38	18	1
1:A:53:SER:HB2	1:A:79:ILE:HD12	0.47	1.86	3	1
1:A:79:ILE:HG23	1:B:283:ILE:HG12	0.47	1.85	5	1
1:B:303:ASN:CA	1:B:324:ILE:HD12	0.47	2.40	8	2
1:A:17:VAL:HG21	1:A:27:THR:HG22	0.47	1.87	9	1
1:A:24:LEU:HD11	1:B:299:THR:CG2	0.47	2.26	4	1
1:B:247:VAL:HG21	1:B:290:LEU:HD22	0.47	1.86	14	1
1:A:17:VAL:HG13	1:A:29:SER:HB2	0.47	1.86	19	1
1:B:232:LEU:HD23	1:B:248:SER:O	0.47	2.09	1	1
1:A:125:VAL:HG22	1:A:126:SER:N	0.47	2.25	20	2
1:B:215:LYS:C	1:B:216:ILE:HD12	0.47	2.29	11	1
1:B:250:GLN:HB3	1:B:282:VAL:HA	0.47	1.85	12	1
1:A:24:LEU:HB3	1:A:26:THR:HG23	0.47	1.86	7	2
1:B:250:GLN:HE21	1:B:283:ILE:HD12	0.47	1.68	12	1
1:A:26:THR:HG21	1:A:55:TYR:CG	0.47	2.44	13	2
1:A:93:LEU:HD13	1:A:93:LEU:C	0.47	2.31	2	3
1:B:224:LEU:HB3	1:B:226:THR:HG23	0.47	1.87	10	1
1:A:77:GLN:OE1	1:A:79:ILE:HD11	0.47	2.10	11	1
1:B:250:GLN:CG	1:B:282:VAL:HA	0.47	2.40	12	1
1:A:111:GLY:CA	1:A:118:LEU:HD13	0.46	2.41	20	1
1:B:244:LEU:HD21	1:B:288:GLU:OE2	0.46	2.10	7	1
1:A:107:LEU:O	1:A:107:LEU:HD13	0.46	2.10	8	2
1:B:303:ASN:O	1:B:307:LEU:HD23	0.46	2.10	11	1
1:A:55:TYR:O	1:A:56:LYS:O	0.46	2.34	18	1
1:B:307:LEU:HD23	1:B:324:ILE:HD13	0.46	1.86	20	1
1:A:45:ASN:O	1:A:87:ALA:HB2	0.46	2.10	4	1
1:A:92:THR:HG21	1:B:255:TYR:CE1	0.46	2.45	13	1
1:A:83:ILE:HG21	1:A:93:LEU:CD2	0.46	2.40	14	2
1:A:52:VAL:HG11	1:A:80:ARG:HA	0.46	1.86	19	1
1:A:51:TYR:CD2	1:A:51:TYR:C	0.46	2.88	6	2
1:B:300:HIS:NE2	1:B:304:VAL:HG21	0.46	2.25	16	1
1:A:53:SER:OG	1:A:79:ILE:HD12	0.46	2.11	18	1
1:A:90:LEU:C	1:A:90:LEU:CD2	0.46	2.70	1	1
1:A:19:SER:CB	1:A:27:THR:HG23	0.46	2.40	11	2
1:A:100:HIS:CD2	1:B:279:ILE:HG21	0.46	2.46	17	1
1:A:55:TYR:CD1	1:A:55:TYR:N	0.46	2.79	16	1
1:B:219:SER:OG	1:B:226:THR:HG23	0.46	2.09	7	1
1:A:102:ARG:HG3	1:A:125:VAL:HG23	0.46	1.88	3	1
1:B:250:GLN:HG2	1:B:282:VAL:HG22	0.46	1.88	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:22:THR:O	1:A:23:ARG:C	0.46	2.54	14	5
1:B:255:TYR:N	1:B:255:TYR:CD1	0.46	2.84	8	2
1:A:93:LEU:HD13	1:A:93:LEU:O	0.45	2.11	14	1
1:A:55:TYR:CD1	1:A:55:TYR:O	0.45	2.69	16	1
1:B:303:ASN:ND2	1:B:304:VAL:HG23	0.45	2.26	17	1
1:B:307:LEU:HD23	1:B:324:ILE:CD1	0.45	2.41	3	1
1:A:108:PHE:CE1	1:B:293:LEU:HD12	0.45	2.47	8	1
1:A:83:ILE:HG21	1:A:93:LEU:CD1	0.45	2.38	16	1
1:B:219:SER:HB2	1:B:227:THR:HG23	0.45	1.88	20	1
1:B:222:THR:O	1:B:223:ARG:C	0.45	2.54	14	5
1:A:100:HIS:CD2	1:A:100:HIS:C	0.45	2.90	9	2
1:A:75:GLU:HG3	1:B:244:LEU:HD21	0.45	1.87	12	1
1:A:55:TYR:HB2	1:A:77:GLN:HB3	0.45	1.89	18	1
1:B:216:ILE:HD11	1:B:230:ALA:HB3	0.45	1.88	4	1
1:B:299:THR:HG22	1:B:327:SER:CB	0.45	2.41	8	1
1:A:23:ARG:C	1:A:24:LEU:HD22	0.45	2.31	14	1
1:A:23:ARG:CD	1:A:24:LEU:H	0.45	2.25	15	1
1:B:228:PHE:HB3	1:B:253:SER:HA	0.45	1.88	17	3
1:A:44:LEU:HD21	1:B:275:GLU:HG3	0.45	1.87	12	1
1:A:81:THR:HG22	1:A:83:ILE:HD11	0.45	1.88	14	1
1:A:92:THR:HG22	1:A:96:GLU:CG	0.45	2.42	1	1
1:A:93:LEU:HD22	1:A:93:LEU:C	0.45	2.33	2	2
1:B:244:LEU:HD23	1:B:288:GLU:OE2	0.45	2.12	13	1
1:A:102:ARG:HG2	1:A:103:ASN:N	0.45	2.27	8	2
1:B:281:THR:HG22	1:B:283:ILE:HD11	0.45	1.89	14	1
1:A:44:LEU:CD1	1:A:87:ALA:HB3	0.45	2.41	20	1
1:B:293:LEU:C	1:B:293:LEU:HD13	0.44	2.32	4	7
1:A:28:PHE:CE1	1:A:30:ALA:HB2	0.44	2.47	3	1
1:A:107:LEU:HD23	1:A:124:ILE:CD1	0.44	2.41	20	2
1:A:113:ALA:HB3	1:B:247:VAL:CG1	0.44	2.42	17	1
1:A:77:GLN:HG2	1:B:292:THR:HG21	0.44	1.89	19	1
1:A:32:LEU:HD11	1:A:48:SER:O	0.44	2.11	4	1
1:B:245:ASN:O	1:B:287:ALA:HB2	0.44	2.11	4	1
1:A:90:LEU:HD12	1:A:90:LEU:C	0.44	2.33	8	2
1:A:83:ILE:HG21	1:A:93:LEU:HD21	0.44	1.89	14	1
1:A:47:VAL:CG1	1:B:313:ALA:HB3	0.44	2.42	17	1
1:A:32:LEU:HD11	1:A:34:ARG:HB2	0.44	1.88	16	1
1:A:112:ASN:OD1	1:A:115:LEU:HD22	0.44	2.12	20	1
1:A:97:TRP:CE2	1:B:304:VAL:HG11	0.44	2.48	8	1
1:B:218:TRP:CZ3	1:B:230:ALA:HB3	0.44	2.48	3	1
1:A:118:LEU:HD13	1:A:119:ASP:N	0.44	2.27	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:217:VAL:HG12	1:B:229:SER:HB3	0.44	1.89	5	1
1:A:17:VAL:HG21	1:A:54:VAL:CG2	0.44	2.42	16	1
1:A:32:LEU:HG	1:B:313:ALA:HB1	0.44	1.89	19	1
1:B:227:THR:O	1:B:254:VAL:CG1	0.44	2.62	20	1
1:B:250:GLN:CB	1:B:282:VAL:HG12	0.44	2.43	20	1
1:A:93:LEU:HD12	1:B:308:PHE:CE1	0.44	2.47	8	1
1:B:217:VAL:O	1:B:217:VAL:HG23	0.44	2.12	15	1
1:A:83:ILE:HG22	1:A:89:ASN:HD21	0.43	1.73	11	2
1:A:102:ARG:CZ	1:A:102:ARG:HB2	0.43	2.42	16	1
1:A:81:THR:OG1	1:B:281:THR:HG23	0.43	2.12	18	1
1:A:104:VAL:HG11	1:B:297:TRP:CE2	0.43	2.48	8	1
1:A:114:GLY:O	1:A:115:LEU:HD13	0.43	2.14	20	2
1:B:293:LEU:HD22	1:B:296:GLU:OE2	0.43	2.12	17	1
1:A:52:VAL:CG2	1:A:80:ARG:HA	0.43	2.37	19	1
1:A:80:ARG:HB3	1:B:282:VAL:HG23	0.43	1.89	8	1
1:B:259:ALA:HB2	1:B:273:PRO:HG2	0.43	1.89	9	1
1:A:47:VAL:HG22	1:B:314:GLY:HA2	0.43	1.90	11	1
1:A:102:ARG:CD	1:A:102:ARG:C	0.43	2.86	16	1
1:A:32:LEU:CD1	1:A:32:LEU:N	0.43	2.81	19	1
1:B:217:VAL:HG13	1:B:229:SER:N	0.43	2.28	3	1
1:A:55:TYR:CE2	1:B:292:THR:HG21	0.43	2.49	9	1
1:A:106:THR:CB	1:A:124:ILE:HD13	0.43	2.44	9	3
1:B:250:GLN:HB2	1:B:282:VAL:HA	0.43	1.89	12	1
1:A:17:VAL:O	1:A:17:VAL:HG13	0.43	2.13	16	1
1:A:93:LEU:C	1:A:93:LEU:HD13	0.43	2.34	8	6
1:B:244:LEU:HD23	1:B:287:ALA:HB3	0.43	1.88	9	1
1:B:292:THR:HG22	1:B:296:GLU:OE2	0.43	2.13	14	1
1:A:24:LEU:O	1:A:25:SER:CB	0.43	2.67	15	2
1:A:54:VAL:HG22	1:A:78:SER:HB2	0.43	1.89	19	1
1:B:226:THR:HG21	1:B:255:TYR:CD1	0.43	2.49	19	1
1:A:125:VAL:CG2	1:A:126:SER:N	0.43	2.82	20	2
1:B:226:THR:HG22	1:B:255:TYR:CB	0.43	2.43	18	2
1:A:102:ARG:HH11	1:A:125:VAL:HG23	0.43	1.72	6	1
1:A:24:LEU:HD13	1:A:55:TYR:OH	0.43	2.14	13	1
1:A:107:LEU:HD11	1:A:118:LEU:HD23	0.43	1.91	16	1
1:A:44:LEU:HD11	1:A:86:SER:HB2	0.43	1.91	19	1
1:A:75:GLU:HG2	1:B:244:LEU:HD21	0.42	1.91	12	1
1:B:252:VAL:HG12	1:B:280:ARG:CA	0.42	2.41	14	1
1:B:307:LEU:HD21	1:B:318:LEU:CD2	0.42	2.42	16	1
1:A:103:ASN:ND2	1:A:104:VAL:HG23	0.42	2.28	17	1
1:A:82:VAL:C	1:A:83:ILE:HD12	0.42	2.35	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:92:THR:HG21	1:B:255:TYR:CD2	0.42	2.49	9	2
1:A:33:LEU:HD23	1:A:50:GLN:OE1	0.42	2.13	13	1
1:A:20:ASP:CB	1:A:23:ARG:HG2	0.42	2.43	17	1
1:B:219:SER:HB3	1:B:227:THR:HG22	0.42	1.90	17	1
1:A:18:TRP:CZ3	1:A:30:ALA:HB3	0.42	2.49	3	1
1:A:97:TRP:CH2	1:B:304:VAL:HG21	0.42	2.50	11	1
1:A:115:LEU:HD13	1:A:117:PHE:CE1	0.42	2.49	12	1
1:B:293:LEU:HD13	1:B:293:LEU:C	0.42	2.35	18	2
1:A:17:VAL:HG12	1:A:28:PHE:N	0.42	2.30	19	1
1:B:232:LEU:HD12	1:B:232:LEU:O	0.42	2.14	9	1
1:B:250:GLN:CD	1:B:282:VAL:HG22	0.42	2.35	9	1
1:B:244:LEU:HD21	1:B:286:SER:HB3	0.42	1.91	19	1
1:A:113:ALA:HB1	1:B:247:VAL:CG1	0.42	2.41	20	1
1:A:79:ILE:HD11	1:B:296:GLU:OE2	0.42	2.15	17	1
1:B:312:ASN:OD1	1:B:315:LEU:HD22	0.42	2.14	20	1
1:B:252:VAL:HG23	1:B:280:ARG:HB2	0.42	1.90	7	1
1:B:216:ILE:HD12	1:B:218:TRP:CZ3	0.42	2.49	9	1
1:A:24:LEU:O	1:A:26:THR:HG23	0.42	2.14	9	2
1:B:228:PHE:CE1	1:B:230:ALA:HB2	0.42	2.50	3	1
1:A:16:ILE:O	1:A:29:SER:HA	0.42	2.14	5	1
1:A:118:LEU:HD12	1:A:122:ALA:CB	0.42	2.43	6	1
1:B:228:PHE:CD1	1:B:252:VAL:HG23	0.42	2.50	14	1
1:A:44:LEU:HD12	1:A:87:ALA:HB3	0.42	1.90	20	1
1:B:283:ILE:HG22	1:B:289:ASN:HD21	0.42	1.74	11	1
1:B:253:SER:HB2	1:B:279:ILE:HD12	0.42	1.92	3	1
1:A:17:VAL:HG12	1:A:29:SER:HB3	0.42	1.92	5	1
1:A:44:LEU:HD23	1:A:88:GLU:OE2	0.42	2.14	13	1
1:B:306:THR:CB	1:B:324:ILE:HD13	0.42	2.44	9	2
1:B:254:VAL:O	1:B:254:VAL:HG13	0.42	2.14	11	1
1:A:127:SER:O	1:A:128:ASP:CB	0.42	2.67	14	1
1:A:32:LEU:HD13	1:A:32:LEU:C	0.42	2.34	16	1
1:A:112:ASN:HB2	1:A:115:LEU:HD21	0.42	1.92	16	1
1:B:232:LEU:N	1:B:232:LEU:CD1	0.42	2.82	19	1
1:A:114:GLY:HA2	1:B:247:VAL:HG22	0.41	1.91	11	1
1:A:28:PHE:HE1	1:A:30:ALA:HB2	0.41	1.74	3	1
1:B:325:VAL:HG22	1:B:326:SER:N	0.41	2.31	17	1
1:A:32:LEU:HD22	1:B:316:GLY:HA2	0.41	1.91	2	1
1:A:113:ALA:HB3	1:B:247:VAL:HG23	0.41	1.91	4	1
1:A:115:LEU:HD13	1:A:115:LEU:N	0.41	2.30	11	1
1:B:216:ILE:HD11	1:B:230:ALA:O	0.41	2.15	8	1
1:B:289:ASN:OD1	1:B:289:ASN:C	0.41	2.59	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:300:HIS:CE1	1:B:304:VAL:HG21	0.41	2.50	16	1
1:A:47:VAL:HG11	1:A:90:LEU:CD2	0.41	2.46	5	1
1:A:96:GLU:CD	1:B:279:ILE:HD12	0.41	2.35	1	1
1:B:302:ARG:HE	1:B:325:VAL:HG23	0.41	1.75	1	1
1:B:308:PHE:CD2	1:B:308:PHE:C	0.41	2.93	5	1
1:A:87:ALA:O	1:A:90:LEU:HD23	0.41	2.16	8	1
1:A:23:ARG:CG	1:A:24:LEU:H	0.41	2.28	15	1
1:A:23:ARG:HG3	1:A:24:LEU:N	0.41	2.30	17	1
1:A:96:GLU:HA	1:A:99:THR:OG1	0.41	2.15	4	1
1:B:282:VAL:C	1:B:283:ILE:HD12	0.41	2.36	9	1
1:A:93:LEU:C	1:A:93:LEU:HD23	0.41	2.35	16	1
1:A:111:GLY:HA2	1:A:118:LEU:HD13	0.41	1.90	20	1
1:B:224:LEU:O	1:B:226:THR:HG23	0.41	2.16	3	1
1:B:228:PHE:HE1	1:B:230:ALA:HB2	0.41	1.75	3	1
1:A:126:SER:OG	1:B:224:LEU:HD11	0.41	2.16	2	1
1:A:50:GLN:HB2	1:A:82:VAL:HG12	0.41	1.91	20	2
1:A:55:TYR:HB2	1:A:77:GLN:N	0.41	2.31	16	1
1:A:24:LEU:HD13	1:A:55:TYR:CD2	0.41	2.51	17	1
1:B:217:VAL:HG23	1:B:228:PHE:CA	0.41	2.45	17	1
1:B:232:LEU:H	1:B:232:LEU:HD13	0.41	1.75	19	1
1:A:90:LEU:O	1:A:90:LEU:HD23	0.41	2.16	3	1
1:B:307:LEU:O	1:B:307:LEU:HD13	0.40	2.16	8	1
1:A:28:PHE:CE2	1:A:52:VAL:HB	0.40	2.51	1	1
1:A:32:LEU:N	1:A:32:LEU:HD13	0.40	2.31	19	1
1:A:32:LEU:H	1:A:32:LEU:HD13	0.40	1.76	19	1
1:B:226:THR:HG21	1:B:255:TYR:HD1	0.40	1.75	19	1
1:A:115:LEU:N	1:A:115:LEU:HD23	0.40	2.32	10	1
1:B:224:LEU:CB	1:B:226:THR:HG23	0.40	2.47	10	1
1:B:231:SER:H	1:B:251:TYR:HB2	0.40	1.76	12	1
1:A:124:ILE:CG2	1:A:125:VAL:N	0.40	2.84	16	1
1:B:293:LEU:C	1:B:293:LEU:HD23	0.40	2.36	10	1
1:A:32:LEU:HD22	1:B:316:GLY:O	0.40	2.16	13	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	99/131 (76%)	87±2 (88±2%)	9±2 (10±2%)	2±1 (2±1%)	9 46
1	B	99/131 (76%)	87±2 (88±2%)	10±2 (10±2%)	2±1 (2±1%)	10 49
All	All	3960/5240 (76%)	3488 (88%)	381 (10%)	91 (2%)	9 48

All 19 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	B	286	SER	12
1	A	86	SER	10
1	A	127	SER	9
1	B	327	SER	9
1	B	223	ARG	7
1	A	23	ARG	6
1	A	35	GLN	6
1	A	15	LYS	5
1	B	215	LYS	5
1	A	128	ASP	4
1	A	122	ALA	4
1	B	328	ASP	3
1	B	322	ALA	3
1	B	235	GLN	3
1	A	4	LYS	1
1	A	26	THR	1
1	B	217	VAL	1
1	A	56	LYS	1
1	A	52	VAL	1

6.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	85/109 (78%)	57±5 (68±6%)	28±5 (32±6%)	1 12
1	B	85/109 (78%)	58±5 (68±5%)	27±5 (32±5%)	1 14
All	All	3400/4360 (78%)	2313 (68%)	1087 (32%)	1 13

All 143 unique residues with a non-rotameric sidechain are listed below. They are sorted by the

frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	115	LEU	20
1	B	315	LEU	20
1	A	25	SER	16
1	A	27	THR	16
1	A	107	LEU	16
1	B	307	LEU	16
1	A	32	LEU	15
1	B	225	SER	15
1	A	29	SER	15
1	B	229	SER	15
1	A	72	MET	15
1	B	272	MET	15
1	B	227	THR	14
1	A	126	SER	13
1	B	326	SER	13
1	A	23	ARG	13
1	A	57	ARG	13
1	A	78	SER	13
1	A	86	SER	13
1	B	278	SER	13
1	B	286	SER	13
1	A	35	GLN	12
1	A	117	PHE	12
1	A	118	LEU	12
1	B	232	LEU	12
1	B	317	PHE	12
1	B	318	LEU	12
1	B	257	ARG	12
1	A	7	GLN	12
1	A	53	SER	11
1	A	128	ASP	11
1	B	235	GLN	11
1	B	253	SER	11
1	A	119	ASP	11
1	B	234	ARG	11
1	B	319	ASP	11
1	B	207	GLN	11
1	A	20	ASP	10
1	B	222	THR	10
1	B	256	LYS	10
1	B	277	GLN	10
1	B	328	ASP	10

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Mol	Chain	Res	Type	Models (Total)
1	A	103	ASN	10
1	B	223	ARG	10
1	A	84	SER	10
1	B	284	SER	10
1	A	22	THR	9
1	A	56	LYS	9
1	A	77	GLN	9
1	A	90	LEU	9
1	A	97	TRP	9
1	A	98	GLU	9
1	A	101	LYS	9
1	B	219	SER	9
1	B	298	GLU	9
1	A	34	ARG	9
1	B	206	MET	9
1	B	301	LYS	9
1	B	303	ASN	9
1	A	4	LYS	9
1	B	204	LYS	9
1	B	228	PHE	9
1	B	297	TRP	8
1	A	6	MET	8
1	B	215	LYS	8
1	A	31	SER	8
1	A	48	SER	8
1	B	231	SER	8
1	A	33	LEU	8
1	A	28	PHE	7
1	A	108	PHE	7
1	B	305	ASP	7
1	B	308	PHE	7
1	A	19	SER	7
1	A	44	LEU	7
1	B	244	LEU	7
1	B	248	SER	7
1	B	233	LEU	7
1	A	15	LYS	7
1	A	52	VAL	7
1	B	246	ASN	7
1	A	45	ASN	6
1	B	220	ASP	6
1	B	245	ASN	6

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Mol	Chain	Res	Type	Models (Total)
1	B	290	LEU	6
1	B	252	VAL	6
1	B	274	ASN	6
1	B	276	ASN	6
1	A	46	ASN	6
1	A	51	TYR	5
1	A	93	LEU	5
1	A	105	ASP	5
1	B	251	TYR	5
1	A	74	ASN	5
1	A	75	GLU	5
1	B	275	GLU	5
1	B	281	THR	5
1	A	94	LYS	5
1	B	294	LYS	5
1	A	102	ARG	5
1	A	124	ILE	5
1	B	324	ILE	5
1	B	218	TRP	5
1	A	88	GLU	5
1	B	288	GLU	5
1	B	224	LEU	4
1	B	250	GLN	4
1	B	293	LEU	4
1	A	80	ARG	4
1	B	280	ARG	4
1	A	81	THR	4
1	A	127	SER	4
1	A	76	ASN	4
1	A	24	LEU	3
1	A	18	TRP	3
1	A	110	SER	3
1	B	216	ILE	3
1	B	327	SER	3
1	A	100	HIS	3
1	A	92	THR	3
1	B	226	THR	3
1	A	50	GLN	2
1	A	16	ILE	2
1	B	310	SER	2
1	B	300	HIS	2
1	B	302	ARG	2

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Mol	Chain	Res	Type	Models (Total)
1	A	82	VAL	2
1	A	89	ASN	2
1	A	17	VAL	2
1	B	292	THR	2
1	A	55	TYR	2
1	A	26	THR	2
1	A	47	VAL	1
1	B	282	VAL	1
1	B	289	ASN	1
1	A	54	VAL	1
1	A	121	THR	1
1	A	96	GLU	1
1	A	112	ASN	1
1	B	247	VAL	1
1	B	312	ASN	1
1	B	254	VAL	1
1	B	321	THR	1

6.3.3 RNA

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates

There are no monosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 35% for the well-defined parts and 30% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *AP205_BMRB.str*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1021
Number of shifts mapped to atoms	1021
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	8

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	110	-0.03 ± 0.17	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	97	0.26 ± 0.13	None needed (< 0.5 ppm)
$^{13}C'$	101	0.08 ± 0.13	None needed (< 0.5 ppm)
^{15}N	100	-0.49 ± 0.39	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 35%, i.e. 919 atoms were assigned a chemical shift out of a possible 2624. 0 out of 32 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	455/976 (47%)	185/394 (47%)	184/396 (46%)	86/186 (46%)
Sidechain	460/1490 (31%)	305/972 (31%)	155/456 (34%)	0/62 (0%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	4/158 (3%)	3/78 (4%)	0/74 (0%)	1/6 (17%)
Overall	919/2624 (35%)	493/1444 (34%)	339/926 (37%)	87/254 (34%)

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 30%, i.e. 1018 atoms were assigned a chemical shift out of a possible 3400. 0 out of 38 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	520/1292 (40%)	211/522 (40%)	211/524 (40%)	98/246 (40%)
Sidechain	494/1950 (25%)	327/1276 (26%)	167/598 (28%)	0/76 (0%)
Aromatic	4/158 (3%)	3/78 (4%)	0/74 (0%)	1/6 (17%)
Overall	1018/3400 (30%)	541/1876 (29%)	378/1196 (32%)	99/328 (30%)

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

7.1.4 Statistically unusual chemical shifts (i)

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

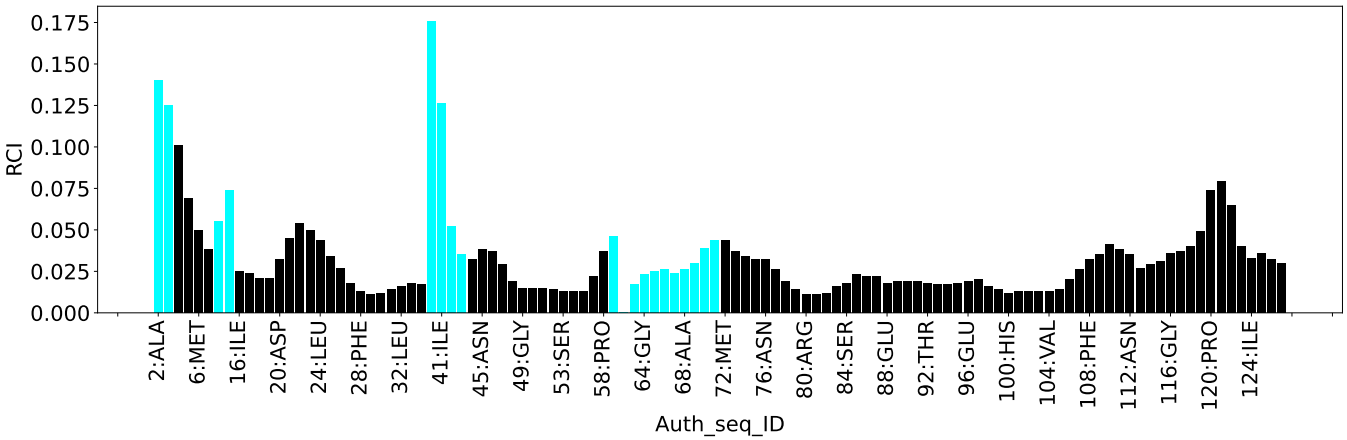
List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	106	THR	HG1	5.89	0.08 – 2.19	22.5
1	A	83	ILE	HD11	-1.19	-0.72 – 2.09	-6.7
1	A	83	ILE	HD12	-1.19	-0.72 – 2.09	-6.7
1	A	83	ILE	HD13	-1.19	-0.72 – 2.09	-6.7
1	A	103	ASN	HB2	0.79	1.27 – 4.34	-6.6
1	A	104	VAL	HG11	-0.80	-0.48 – 2.12	-6.2
1	A	104	VAL	HG12	-0.80	-0.48 – 2.12	-6.2
1	A	104	VAL	HG13	-0.80	-0.48 – 2.12	-6.2

7.1.5 Random Coil Index (RCI) plots (i)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble

composition.If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



8 NMR restraints analysis

8.1 Conformationally restricting restraints

The following table provides the summary of experimentally observed NMR restraints in different categories. Restraints are classified into different categories based on the sequence separation of the atoms involved.

Description	Value
Total distance restraints	1312
Intra-residue (|i-j|=0)	144
Sequential (|i-j|=1)	542
Medium range (|i-j|>1 and |i-j|<5)	248
Long range (|i-j|≥5)	288
Inter-chain	90
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	5.0
Number of long range restraints per residue[1]	1.1

[1]Long range hydrogen bonds and disulfide bonds are counted as long range restraints while calculating the number of long range restraints per residue

8.2 Residual restraint violations

This section provides the overview of the restraint violations analysis. The violations are binned as small, medium and large violations based on its absolute value. Average number of violations per model is calculated by dividing the total number of violations in each bin by the size of the ensemble.

8.2.1 Average number of distance violations per model

Distance violations less than 0.1 Å are not included in the calculation.

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	17.3	0.2
0.2-0.5 (Medium)	22.8	0.5
>0.5 (Large)	43.6	2.48

8.2.2 Average number of dihedral-angle violations per model (i)

Dihedral-angle violations less than 1° are not included in the calculation.There are no dihedral-angle violations

9 Distance violation analysis (i)

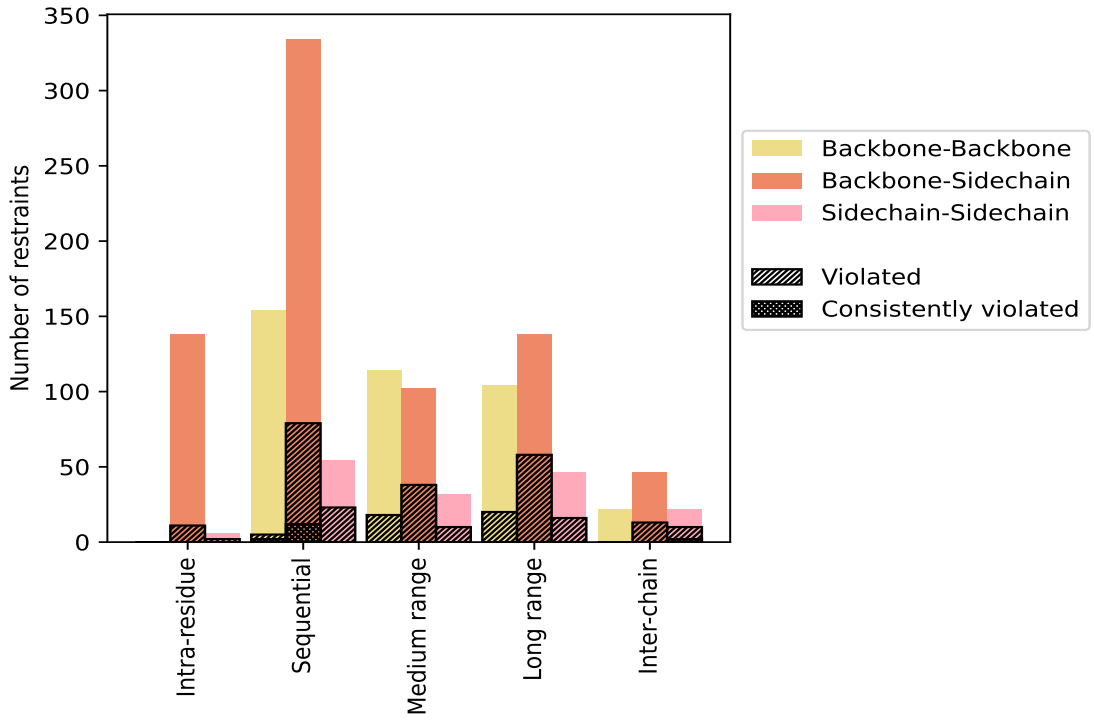
9.1 Summary of distance violations (i)

The following table shows the summary of distance violations in different restraint categories based on the sequence separation of the atoms involved. Each category is further sub-divided into three sub-categories based on the atoms involved. Violations less than 0.1 Å are not included in the statistics.

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	144	11.0	13	9.0	1.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	138	10.5	11	8.0	0.8	0	0.0	0.0
Sidechain-Sidechain	6	0.5	2	33.3	0.2	0	0.0	0.0
Sequential (|i-j|=1)	542	41.3	107	19.7	8.2	14	2.6	1.1
Backbone-Backbone	154	11.7	5	3.2	0.4	2	1.3	0.2
Backbone-Sidechain	334	25.5	79	23.7	6.0	12	3.6	0.9
Sidechain-Sidechain	54	4.1	23	42.6	1.8	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	248	18.9	66	26.6	5.0	0	0.0	0.0
Backbone-Backbone	114	8.7	18	15.8	1.4	0	0.0	0.0
Backbone-Sidechain	102	7.8	38	37.3	2.9	0	0.0	0.0
Sidechain-Sidechain	32	2.4	10	31.2	0.8	0	0.0	0.0
Long range (|i-j|≥5)	288	22.0	94	32.6	7.2	0	0.0	0.0
Backbone-Backbone	104	7.9	20	19.2	1.5	0	0.0	0.0
Backbone-Sidechain	138	10.5	58	42.0	4.4	0	0.0	0.0
Sidechain-Sidechain	46	3.5	16	34.8	1.2	0	0.0	0.0
Inter-chain	90	6.9	23	25.6	1.8	2	2.2	0.2
Backbone-Backbone	22	1.7	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	46	3.5	13	28.3	1.0	0	0.0	0.0
Sidechain-Sidechain	22	1.7	10	45.5	0.8	2	9.1	0.2
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1312	100.0	303	23.1	23.1	16	1.2	1.2
Backbone-Backbone	394	30.0	43	10.9	3.3	2	0.5	0.2
Backbone-Sidechain	758	57.8	199	26.3	15.2	12	1.6	0.9
Sidechain-Sidechain	160	12.2	61	38.1	4.6	2	1.2	0.2

[1] percentage calculated with respect to the total number of distance restraints, [2] percentage calculated with respect to the number of restraints in a particular restraint category, [3] violated in at least one model, [4] violated in all the models

9.1.1 Bar chart : Distribution of distance restraints and violations



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfied bonds are counted in their appropriate category on the x-axis

9.2 Distance violation statistics for each model

The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	4	43	16	24	5	92	0.69	2.04	0.52	0.54
2	0	36	19	17	4	76	0.74	2.39	0.56	0.64
3	4	33	16	12	6	71	0.66	2.16	0.5	0.5
4	3	34	20	15	5	77	0.76	2.04	0.55	0.62
5	2	45	18	13	6	84	0.71	1.96	0.55	0.59
6	2	35	13	20	5	75	0.66	1.94	0.46	0.6
7	0	31	16	14	4	65	0.83	2.29	0.52	0.84
8	0	33	13	26	9	81	0.68	1.91	0.46	0.56
9	2	32	14	17	5	70	0.69	2.08	0.49	0.59
10	4	38	22	16	7	87	0.74	2.32	0.53	0.72
11	4	39	26	17	6	92	0.7	2.05	0.52	0.57

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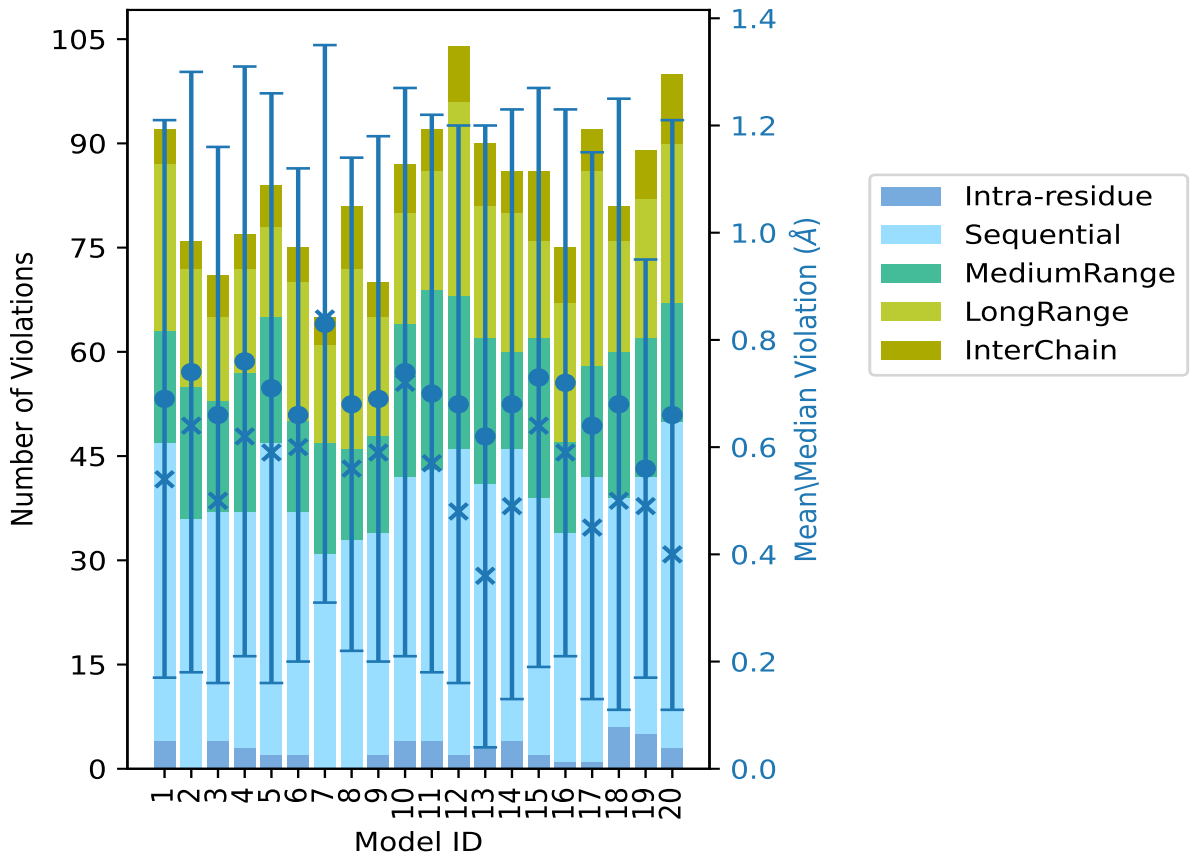
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	2	44	22	28	8	104	0.68	2.17	0.52	0.48
13	3	38	21	19	9	90	0.62	2.48	0.58	0.36
14	4	42	14	20	6	86	0.68	2.2	0.55	0.49
15	2	37	23	14	10	86	0.73	2.2	0.54	0.64
16	1	33	13	20	8	75	0.72	2.44	0.51	0.59
17	1	41	16	28	6	92	0.64	2.15	0.51	0.45
18	6	33	21	16	5	81	0.68	2.2	0.57	0.5
19	5	37	20	20	7	89	0.56	1.85	0.39	0.49
20	3	47	17	23	10	100	0.66	2.28	0.55	0.4

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6]Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model



The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis on the right

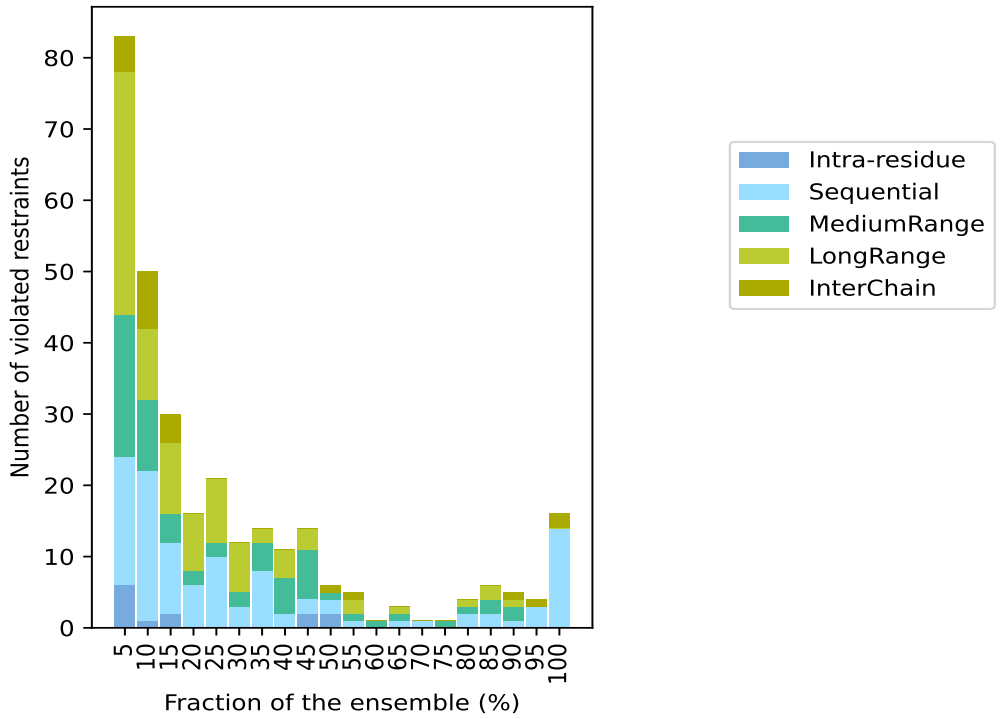
9.3 Distance violation statistics for the ensemble (i)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 1009(IR:131, SQ:435, MR:182, LR:194, IC:67) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
6	18	20	34	5	83	1	5.0
1	21	10	10	8	50	2	10.0
2	10	4	10	4	30	3	15.0
0	6	2	8	0	16	4	20.0
0	10	2	9	0	21	5	25.0
0	3	2	7	0	12	6	30.0
0	8	4	2	0	14	7	35.0
0	2	5	4	0	11	8	40.0
2	2	7	3	0	14	9	45.0
2	2	1	0	1	6	10	50.0
0	1	1	2	1	5	11	55.0
0	0	1	0	0	1	12	60.0
0	1	1	1	0	3	13	65.0
0	1	0	0	0	1	14	70.0
0	0	1	0	0	1	15	75.0
0	2	1	1	0	4	16	80.0
0	2	2	2	0	6	17	85.0
0	1	2	1	1	5	18	90.0
0	3	0	0	1	4	19	95.0
0	14	0	0	2	16	20	100.0

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6] Number of models with violations

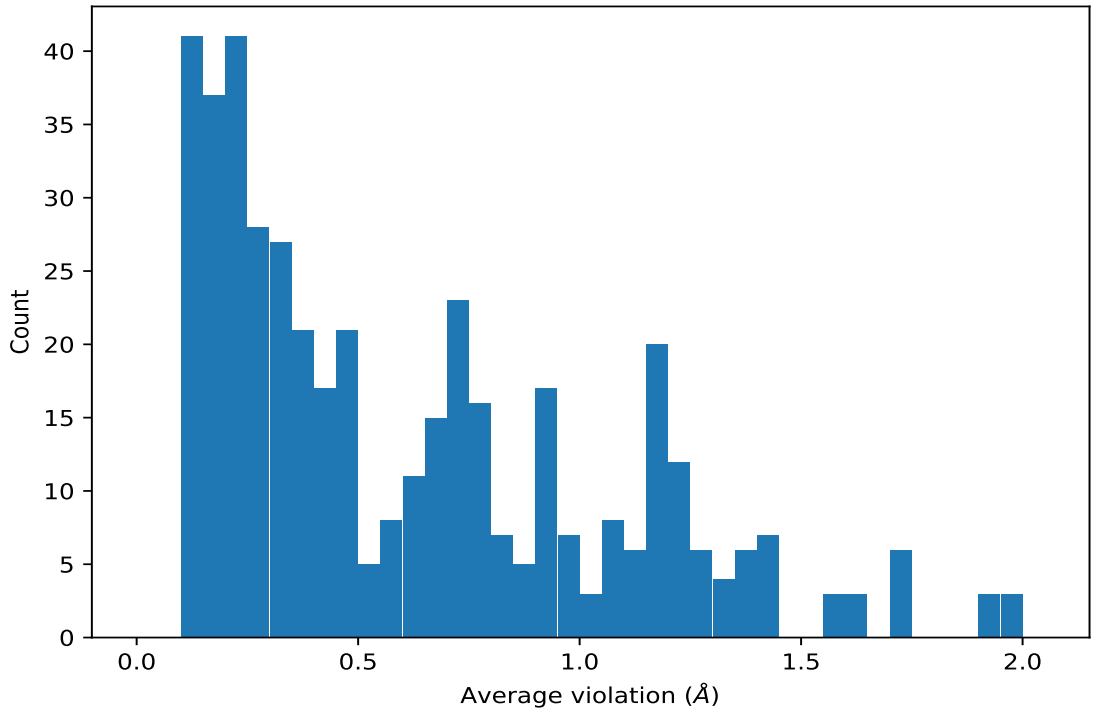
9.3.1 Bar graph : Distance violation statistics for the ensemble



9.4 Most violated distance restraints in the ensemble

9.4.1 Histogram : Distribution of mean distance violations

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models in the ensemble



9.4.2 Table: Most violated distance restraints

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,610)	1:B:249:GLY:HA3	1:B:250:GLN:HB2	20	1.16	0.41	1.02
(1,609)	1:A:49:GLY:HA3	1:A:50:GLN:HB2	20	1.1	0.33	1.01
(1,280)	1:B:258:PRO:HB3	1:B:259:ALA:HA	20	1.08	0.08	1.12
(1,279)	1:A:58:PRO:HB3	1:A:59:ALA:HA	20	1.07	0.08	1.12
(1,513)	1:A:5:PRO:HB2	1:B:325:VAL:HB	20	0.93	0.29	0.94
(1,514)	1:A:125:VAL:HB	1:B:205:PRO:HB2	20	0.87	0.35	0.89
(1,61)	1:A:107:LEU:HB2	1:A:108:PHE:HA	20	0.79	0.18	0.76
(1,62)	1:B:307:LEU:HB2	1:B:308:PHE:HA	20	0.79	0.18	0.76
(1,326)	1:A:5:PRO:HB3	1:A:6:MET:HA	20	0.73	0.09	0.73
(1,328)	1:B:205:PRO:HB3	1:B:206:MET:HA	20	0.72	0.08	0.73
(1,298)	1:B:219:SER:HA	1:B:220:ASP:HB3	20	0.69	0.21	0.66
(1,297)	1:A:19:SER:HA	1:A:20:ASP:HB3	20	0.62	0.18	0.62
(1,782)	1:B:315:LEU:H	1:B:316:GLY:HA3	20	0.43	0.05	0.42
(1,781)	1:A:115:LEU:H	1:A:116:GLY:HA3	20	0.42	0.05	0.42
(1,124)	1:B:293:LEU:HB2	1:B:294:LYS:HA	20	0.29	0.05	0.3
(1,123)	1:A:93:LEU:HB2	1:A:94:LYS:HA	20	0.29	0.05	0.3

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,549)	1:B:220:ASP:HB2	1:B:221:PRO:HB2	19	1.14	0.38	1.34
(1,633)	1:A:5:PRO:HB2	1:B:325:VAL:HG21	19	0.78	0.12	0.8
(1,633)	1:A:5:PRO:HB2	1:B:325:VAL:HG22	19	0.78	0.12	0.8
(1,633)	1:A:5:PRO:HB2	1:B:325:VAL:HG23	19	0.78	0.12	0.8
(1,1066)	1:B:282:VAL:H	1:B:283:ILE:HG12	19	0.58	0.14	0.58
(1,1065)	1:A:82:VAL:H	1:A:83:ILE:HG12	19	0.51	0.14	0.53
(1,627)	1:A:52:VAL:HG21	1:A:54:VAL:HA	18	1.71	0.38	1.81
(1,627)	1:A:52:VAL:HG22	1:A:54:VAL:HA	18	1.71	0.38	1.81
(1,627)	1:A:52:VAL:HG23	1:A:54:VAL:HA	18	1.71	0.38	1.81
(1,628)	1:A:52:VAL:HG21	1:A:79:ILE:HA	18	1.18	0.45	1.11
(1,628)	1:A:52:VAL:HG22	1:A:79:ILE:HA	18	1.18	0.45	1.11
(1,628)	1:A:52:VAL:HG23	1:A:79:ILE:HA	18	1.18	0.45	1.11
(1,498)	1:B:220:ASP:HB2	1:B:223:ARG:HD3	18	1.13	0.53	1.1
(1,635)	1:A:125:VAL:HG21	1:B:205:PRO:HB2	18	0.78	0.15	0.78
(1,635)	1:A:125:VAL:HG22	1:B:205:PRO:HB2	18	0.78	0.15	0.78
(1,635)	1:A:125:VAL:HG23	1:B:205:PRO:HB2	18	0.78	0.15	0.78
(1,318)	1:A:74:ASN:HB3	1:A:75:GLU:HA	18	0.33	0.08	0.34
(1,1214)	1:A:31:SER:H	1:A:52:VAL:HG11	17	1.6	0.44	1.79
(1,1214)	1:A:31:SER:H	1:A:52:VAL:HG12	17	1.6	0.44	1.79
(1,1214)	1:A:31:SER:H	1:A:52:VAL:HG13	17	1.6	0.44	1.79
(1,630)	1:B:252:VAL:HG21	1:B:279:ILE:HA	17	1.18	0.43	1.37
(1,630)	1:B:252:VAL:HG22	1:B:279:ILE:HA	17	1.18	0.43	1.37
(1,630)	1:B:252:VAL:HG23	1:B:279:ILE:HA	17	1.18	0.43	1.37
(1,547)	1:A:20:ASP:HB2	1:A:21:PRO:HB2	17	1.16	0.36	1.34
(1,497)	1:A:20:ASP:HB2	1:A:23:ARG:HD3	17	1.08	0.46	1.11
(1,1267)	1:A:17:VAL:HG11	1:A:19:SER:H	17	1.07	0.77	0.82
(1,1267)	1:A:17:VAL:HG12	1:A:19:SER:H	17	1.07	0.77	0.82
(1,1267)	1:A:17:VAL:HG13	1:A:19:SER:H	17	1.07	0.77	0.82
(1,224)	1:B:315:LEU:HD21	1:B:316:GLY:HA2	17	0.93	0.42	0.62
(1,224)	1:B:315:LEU:HD22	1:B:316:GLY:HA2	17	0.93	0.42	0.62
(1,224)	1:B:315:LEU:HD23	1:B:316:GLY:HA2	17	0.93	0.42	0.62
(1,1216)	1:B:231:SER:H	1:B:252:VAL:HG11	16	1.28	0.57	1.28
(1,1216)	1:B:231:SER:H	1:B:252:VAL:HG12	16	1.28	0.57	1.28
(1,1216)	1:B:231:SER:H	1:B:252:VAL:HG13	16	1.28	0.57	1.28
(1,1268)	1:B:217:VAL:HG11	1:B:219:SER:H	16	1.22	0.61	1.11
(1,1268)	1:B:217:VAL:HG12	1:B:219:SER:H	16	1.22	0.61	1.11
(1,1268)	1:B:217:VAL:HG13	1:B:219:SER:H	16	1.22	0.61	1.11
(1,320)	1:B:274:ASN:HB3	1:B:275:GLU:HA	16	0.35	0.05	0.35
(1,607)	1:A:50:GLN:HB2	1:A:51:TYR:HA	16	0.19	0.04	0.18
(1,629)	1:B:252:VAL:HG21	1:B:254:VAL:HA	15	1.7	0.42	1.84
(1,629)	1:B:252:VAL:HG22	1:B:254:VAL:HA	15	1.7	0.42	1.84
(1,629)	1:B:252:VAL:HG23	1:B:254:VAL:HA	15	1.7	0.42	1.84

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,223)	1:A:115:LEU:HD21	1:A:116:GLY:HA2	14	0.91	0.43	0.6
(1,223)	1:A:115:LEU:HD22	1:A:116:GLY:HA2	14	0.91	0.43	0.6
(1,223)	1:A:115:LEU:HD23	1:A:116:GLY:HA2	14	0.91	0.43	0.6
(1,461)	1:A:103:ASN:HA	1:A:105:ASP:HB2	13	0.93	0.38	1.05
(1,315)	1:A:32:LEU:HA	1:A:50:GLN:HB2	13	0.61	0.31	0.45
(1,608)	1:B:250:GLN:HB2	1:B:251:TYR:HA	13	0.19	0.05	0.18
(1,677)	1:A:90:LEU:HD11	1:A:94:LYS:HG2	12	1.41	0.67	1.62
(1,677)	1:A:90:LEU:HD12	1:A:94:LYS:HG2	12	1.41	0.67	1.62
(1,677)	1:A:90:LEU:HD13	1:A:94:LYS:HG2	12	1.41	0.67	1.62
(1,95)	1:A:32:LEU:HD11	1:A:34:ARG:HA	11	1.17	0.48	1.26
(1,95)	1:A:32:LEU:HD12	1:A:34:ARG:HA	11	1.17	0.48	1.26
(1,95)	1:A:32:LEU:HD13	1:A:34:ARG:HA	11	1.17	0.48	1.26
(1,1108)	1:A:75:GLU:H	1:B:244:LEU:HD11	11	0.87	0.43	0.83
(1,1108)	1:A:75:GLU:H	1:B:244:LEU:HD12	11	0.87	0.43	0.83
(1,1108)	1:A:75:GLU:H	1:B:244:LEU:HD13	11	0.87	0.43	0.83
(1,316)	1:B:232:LEU:HA	1:B:250:GLN:HB2	11	0.7	0.37	0.65
(1,153)	1:A:88:GLU:HB2	1:A:89:ASN:HA	11	0.54	0.26	0.69
(1,901)	1:A:103:ASN:H	1:A:125:VAL:HG21	11	0.35	0.36	0.19
(1,901)	1:A:103:ASN:H	1:A:125:VAL:HG22	11	0.35	0.36	0.19
(1,901)	1:A:103:ASN:H	1:A:125:VAL:HG23	11	0.35	0.36	0.19
(1,462)	1:B:303:ASN:HA	1:B:305:ASP:HB2	10	0.98	0.35	1.06
(1,1107)	1:A:44:LEU:HD11	1:B:275:GLU:H	10	0.92	0.38	0.86
(1,1107)	1:A:44:LEU:HD12	1:B:275:GLU:H	10	0.92	0.38	0.86
(1,1107)	1:A:44:LEU:HD13	1:B:275:GLU:H	10	0.92	0.38	0.86
(1,482)	1:B:302:ARG:H	1:B:302:ARG:HD3	10	0.68	0.29	0.78
(1,154)	1:B:288:GLU:HB2	1:B:289:ASN:HA	10	0.57	0.23	0.7
(1,548)	1:A:69:CYS:HB3	1:A:70:VAL:HB	10	0.46	0.46	0.22
(1,742)	1:B:324:ILE:H	1:B:324:ILE:HG12	10	0.39	0.1	0.4
(1,679)	1:B:290:LEU:HD11	1:B:294:LYS:HG2	9	1.58	0.53	1.73
(1,679)	1:B:290:LEU:HD12	1:B:294:LYS:HG2	9	1.58	0.53	1.73
(1,679)	1:B:290:LEU:HD13	1:B:294:LYS:HG2	9	1.58	0.53	1.73
(1,101)	1:A:93:LEU:HD11	1:A:97:TRP:HA	9	1.36	0.49	1.42
(1,101)	1:A:93:LEU:HD12	1:A:97:TRP:HA	9	1.36	0.49	1.42
(1,101)	1:A:93:LEU:HD13	1:A:97:TRP:HA	9	1.36	0.49	1.42
(1,102)	1:B:293:LEU:HD11	1:B:297:TRP:HA	9	1.35	0.53	1.49
(1,102)	1:B:293:LEU:HD12	1:B:297:TRP:HA	9	1.35	0.53	1.49
(1,102)	1:B:293:LEU:HD13	1:B:297:TRP:HA	9	1.35	0.53	1.49
(1,905)	1:B:303:ASN:H	1:B:324:ILE:HG12	9	1.32	0.44	1.41
(1,800)	1:B:312:ASN:H	1:B:315:LEU:HD21	9	1.27	0.6	1.44
(1,800)	1:B:312:ASN:H	1:B:315:LEU:HD22	9	1.27	0.6	1.44
(1,800)	1:B:312:ASN:H	1:B:315:LEU:HD23	9	1.27	0.6	1.44
(1,457)	1:A:102:ARG:HG3	1:A:105:ASP:HB2	9	0.77	0.48	0.68

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1312)	1:B:232:LEU:HD11	1:B:234:ARG:H	9	0.75	0.62	0.69
(1,1312)	1:B:232:LEU:HD12	1:B:234:ARG:H	9	0.75	0.62	0.69
(1,1312)	1:B:232:LEU:HD13	1:B:234:ARG:H	9	0.75	0.62	0.69
(1,667)	1:A:88:GLU:HB2	1:A:89:ASN:HB2	9	0.74	0.31	0.75
(1,667)	1:A:88:GLU:HB2	1:A:89:ASN:HB3	9	0.74	0.31	0.75
(1,668)	1:B:288:GLU:HB2	1:B:289:ASN:HB2	9	0.7	0.27	0.74
(1,668)	1:B:288:GLU:HB2	1:B:289:ASN:HB3	9	0.7	0.27	0.74
(1,481)	1:A:102:ARG:H	1:A:102:ARG:HD3	9	0.65	0.28	0.77
(1,741)	1:A:124:ILE:H	1:A:124:ILE:HG12	9	0.44	0.06	0.45
(1,1152)	1:B:233:LEU:H	1:B:249:GLY:HA3	9	0.39	0.21	0.28
(1,477)	1:A:108:PHE:HB2	1:A:110:SER:H	9	0.26	0.08	0.27
(1,714)	1:A:103:ASN:HB2	1:A:125:VAL:H	9	0.22	0.07	0.21
(1,34)	1:B:312:ASN:HA	1:B:315:LEU:HD21	8	1.92	0.43	2.08
(1,34)	1:B:312:ASN:HA	1:B:315:LEU:HD22	8	1.92	0.43	2.08
(1,34)	1:B:312:ASN:HA	1:B:315:LEU:HD23	8	1.92	0.43	2.08
(1,97)	1:B:232:LEU:HD11	1:B:234:ARG:HA	8	1.3	0.49	1.34
(1,97)	1:B:232:LEU:HD12	1:B:234:ARG:HA	8	1.3	0.49	1.34
(1,97)	1:B:232:LEU:HD13	1:B:234:ARG:HA	8	1.3	0.49	1.34
(1,1249)	1:A:70:VAL:HG11	1:A:72:MET:H	8	0.92	0.73	0.94
(1,1249)	1:A:70:VAL:HG12	1:A:72:MET:H	8	0.92	0.73	0.94
(1,1249)	1:A:70:VAL:HG13	1:A:72:MET:H	8	0.92	0.73	0.94
(1,1311)	1:A:32:LEU:HD11	1:A:34:ARG:H	8	0.82	0.39	0.78
(1,1311)	1:A:32:LEU:HD12	1:A:34:ARG:H	8	0.82	0.39	0.78
(1,1311)	1:A:32:LEU:HD13	1:A:34:ARG:H	8	0.82	0.39	0.78
(1,588)	1:B:222:THR:H	1:B:223:ARG:HD3	8	0.61	0.52	0.4
(1,1151)	1:A:33:LEU:H	1:A:49:GLY:HA3	8	0.44	0.23	0.36
(1,1260)	1:B:314:GLY:H	1:B:315:LEU:HD21	8	0.43	0.18	0.52
(1,1260)	1:B:314:GLY:H	1:B:315:LEU:HD22	8	0.43	0.18	0.52
(1,1260)	1:B:314:GLY:H	1:B:315:LEU:HD23	8	0.43	0.18	0.52
(1,904)	1:B:303:ASN:H	1:B:325:VAL:HG21	8	0.34	0.46	0.18
(1,904)	1:B:303:ASN:H	1:B:325:VAL:HG22	8	0.34	0.46	0.18
(1,904)	1:B:303:ASN:H	1:B:325:VAL:HG23	8	0.34	0.46	0.18
(1,257)	1:A:17:VAL:HB	1:A:28:PHE:HA	8	0.3	0.14	0.26
(1,478)	1:B:308:PHE:HB2	1:B:310:SER:H	8	0.25	0.08	0.26
(1,716)	1:B:303:ASN:HB2	1:B:325:VAL:H	8	0.2	0.05	0.2
(1,577)	1:A:93:LEU:HD11	1:A:94:LYS:HB2	7	1.23	0.03	1.23
(1,577)	1:A:93:LEU:HD11	1:A:94:LYS:HB3	7	1.23	0.03	1.23
(1,577)	1:A:93:LEU:HD12	1:A:94:LYS:HB2	7	1.23	0.03	1.23
(1,577)	1:A:93:LEU:HD12	1:A:94:LYS:HB3	7	1.23	0.03	1.23
(1,577)	1:A:93:LEU:HD13	1:A:94:LYS:HB2	7	1.23	0.03	1.23
(1,577)	1:A:93:LEU:HD13	1:A:94:LYS:HB3	7	1.23	0.03	1.23
(1,578)	1:B:293:LEU:HD11	1:B:294:LYS:HB2	7	1.15	0.18	1.22

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,578)	1:B:293:LEU:HD11	1:B:294:LYS:HB3	7	1.15	0.18	1.22
(1,578)	1:B:293:LEU:HD12	1:B:294:LYS:HB2	7	1.15	0.18	1.22
(1,578)	1:B:293:LEU:HD12	1:B:294:LYS:HB3	7	1.15	0.18	1.22
(1,578)	1:B:293:LEU:HD13	1:B:294:LYS:HB2	7	1.15	0.18	1.22
(1,578)	1:B:293:LEU:HD13	1:B:294:LYS:HB3	7	1.15	0.18	1.22
(1,902)	1:A:103:ASN:H	1:A:124:ILE:HG12	7	1.07	0.59	1.33
(1,1281)	1:A:93:LEU:HD11	1:A:96:GLU:H	7	1.01	0.2	1.12
(1,1281)	1:A:93:LEU:HD12	1:A:96:GLU:H	7	1.01	0.2	1.12
(1,1281)	1:A:93:LEU:HD13	1:A:96:GLU:H	7	1.01	0.2	1.12
(1,1282)	1:B:293:LEU:HD11	1:B:296:GLU:H	7	0.93	0.21	0.9
(1,1282)	1:B:293:LEU:HD12	1:B:296:GLU:H	7	0.93	0.21	0.9
(1,1282)	1:B:293:LEU:HD13	1:B:296:GLU:H	7	0.93	0.21	0.9
(1,647)	1:A:102:ARG:HG2	1:A:125:VAL:HA	7	0.84	0.66	0.5
(1,550)	1:B:269:CYS:HB3	1:B:270:VAL:HB	7	0.77	0.45	0.75
(1,159)	1:A:87:ALA:HA	1:A:90:LEU:HD21	7	0.69	0.46	0.69
(1,159)	1:A:87:ALA:HA	1:A:90:LEU:HD22	7	0.69	0.46	0.69
(1,159)	1:A:87:ALA:HA	1:A:90:LEU:HD23	7	0.69	0.46	0.69
(1,553)	1:A:24:LEU:HB3	1:A:26:THR:HA	7	0.58	0.29	0.65
(1,657)	1:A:93:LEU:HD11	1:A:94:LYS:HG3	7	0.55	0.28	0.65
(1,657)	1:A:93:LEU:HD12	1:A:94:LYS:HG3	7	0.55	0.28	0.65
(1,657)	1:A:93:LEU:HD13	1:A:94:LYS:HG3	7	0.55	0.28	0.65
(1,636)	1:B:269:CYS:HB2	1:B:270:VAL:HG11	7	0.35	0.09	0.36
(1,636)	1:B:269:CYS:HB2	1:B:270:VAL:HG12	7	0.35	0.09	0.36
(1,636)	1:B:269:CYS:HB2	1:B:270:VAL:HG13	7	0.35	0.09	0.36
(1,634)	1:A:69:CYS:HB2	1:A:70:VAL:HG11	7	0.31	0.13	0.28
(1,634)	1:A:69:CYS:HB2	1:A:70:VAL:HG12	7	0.31	0.13	0.28
(1,634)	1:A:69:CYS:HB2	1:A:70:VAL:HG13	7	0.31	0.13	0.28
(1,118)	1:B:293:LEU:HD11	1:B:294:LYS:HA	7	0.22	0.08	0.17
(1,118)	1:B:293:LEU:HD12	1:B:294:LYS:HA	7	0.22	0.08	0.17
(1,118)	1:B:293:LEU:HD13	1:B:294:LYS:HA	7	0.22	0.08	0.17
(1,200)	1:B:272:MET:H	1:B:273:PRO:HA	7	0.2	0.06	0.19
(1,33)	1:A:112:ASN:HA	1:A:115:LEU:HD21	6	1.96	0.37	2.18
(1,33)	1:A:112:ASN:HA	1:A:115:LEU:HD22	6	1.96	0.37	2.18
(1,33)	1:A:112:ASN:HA	1:A:115:LEU:HD23	6	1.96	0.37	2.18
(1,799)	1:A:112:ASN:H	1:A:115:LEU:HD21	6	1.42	0.44	1.51
(1,799)	1:A:112:ASN:H	1:A:115:LEU:HD22	6	1.42	0.44	1.51
(1,799)	1:A:112:ASN:H	1:A:115:LEU:HD23	6	1.42	0.44	1.51
(1,930)	1:A:50:GLN:H	1:A:82:VAL:HG11	6	1.15	0.13	1.15
(1,930)	1:A:50:GLN:H	1:A:82:VAL:HG12	6	1.15	0.13	1.15
(1,930)	1:A:50:GLN:H	1:A:82:VAL:HG13	6	1.15	0.13	1.15
(1,932)	1:B:250:GLN:H	1:B:282:VAL:HG11	6	1.11	0.1	1.09
(1,932)	1:B:250:GLN:H	1:B:282:VAL:HG12	6	1.11	0.1	1.09

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,932)	1:B:250:GLN:H	1:B:282:VAL:HG13	6	1.11	0.1	1.09
(1,658)	1:B:293:LEU:HD11	1:B:294:LYS:HG3	6	0.77	0.5	0.7
(1,658)	1:B:293:LEU:HD12	1:B:294:LYS:HG3	6	0.77	0.5	0.7
(1,658)	1:B:293:LEU:HD13	1:B:294:LYS:HG3	6	0.77	0.5	0.7
(1,260)	1:B:228:PHE:HA	1:B:252:VAL:HB	6	0.7	0.38	0.56
(1,166)	1:B:244:LEU:HD11	1:B:286:SER:HA	6	0.49	0.23	0.45
(1,166)	1:B:244:LEU:HD12	1:B:286:SER:HA	6	0.49	0.23	0.45
(1,166)	1:B:244:LEU:HD13	1:B:286:SER:HA	6	0.49	0.23	0.45
(1,648)	1:B:302:ARG:HG2	1:B:325:VAL:HA	6	0.49	0.54	0.24
(1,164)	1:A:44:LEU:HD11	1:A:86:SER:HA	6	0.48	0.23	0.45
(1,164)	1:A:44:LEU:HD12	1:A:86:SER:HA	6	0.48	0.23	0.45
(1,164)	1:A:44:LEU:HD13	1:A:86:SER:HA	6	0.48	0.23	0.45
(1,1259)	1:A:114:GLY:H	1:A:115:LEU:HD21	6	0.46	0.16	0.55
(1,1259)	1:A:114:GLY:H	1:A:115:LEU:HD22	6	0.46	0.16	0.55
(1,1259)	1:A:114:GLY:H	1:A:115:LEU:HD23	6	0.46	0.16	0.55
(1,117)	1:A:93:LEU:HD11	1:A:94:LYS:HA	6	0.26	0.08	0.28
(1,117)	1:A:93:LEU:HD12	1:A:94:LYS:HA	6	0.26	0.08	0.28
(1,117)	1:A:93:LEU:HD13	1:A:94:LYS:HA	6	0.26	0.08	0.28
(1,753)	1:A:106:THR:HG21	1:A:123:ALA:H	6	0.13	0.02	0.13
(1,753)	1:A:106:THR:HG22	1:A:123:ALA:H	6	0.13	0.02	0.13
(1,753)	1:A:106:THR:HG23	1:A:123:ALA:H	6	0.13	0.02	0.13
(1,30)	1:B:232:LEU:HD11	1:B:233:LEU:HA	5	0.98	0.48	1.2
(1,30)	1:B:232:LEU:HD12	1:B:233:LEU:HA	5	0.98	0.48	1.2
(1,30)	1:B:232:LEU:HD13	1:B:233:LEU:HA	5	0.98	0.48	1.2
(1,460)	1:B:302:ARG:HG3	1:B:305:ASP:HB2	5	0.88	0.51	0.84
(1,399)	1:A:102:ARG:HG2	1:A:124:ILE:HD11	5	0.65	0.24	0.59
(1,399)	1:A:102:ARG:HG2	1:A:124:ILE:HD12	5	0.65	0.24	0.59
(1,399)	1:A:102:ARG:HG2	1:A:124:ILE:HD13	5	0.65	0.24	0.59
(1,160)	1:B:287:ALA:HA	1:B:290:LEU:HD21	5	0.61	0.4	0.54
(1,160)	1:B:287:ALA:HA	1:B:290:LEU:HD22	5	0.61	0.4	0.54
(1,160)	1:B:287:ALA:HA	1:B:290:LEU:HD23	5	0.61	0.4	0.54
(1,587)	1:A:22:THR:H	1:A:23:ARG:HD3	5	0.56	0.35	0.34
(1,717)	1:A:102:ARG:HG2	1:A:125:VAL:H	5	0.55	0.31	0.64
(1,400)	1:B:302:ARG:HG2	1:B:324:ILE:HD11	5	0.5	0.27	0.47
(1,400)	1:B:302:ARG:HG2	1:B:324:ILE:HD12	5	0.5	0.27	0.47
(1,400)	1:B:302:ARG:HG2	1:B:324:ILE:HD13	5	0.5	0.27	0.47
(1,96)	1:A:70:VAL:HG11	1:A:71:ILE:HA	5	0.39	0.09	0.4
(1,96)	1:A:70:VAL:HG12	1:A:71:ILE:HA	5	0.39	0.09	0.4
(1,96)	1:A:70:VAL:HG13	1:A:71:ILE:HA	5	0.39	0.09	0.4
(1,597)	1:B:249:GLY:H	1:B:250:GLN:HB2	5	0.34	0.17	0.25
(1,307)	1:A:102:ARG:HG2	1:A:103:ASN:HA	5	0.29	0.05	0.28
(1,585)	1:A:75:GLU:HG3	1:A:76:ASN:H	5	0.28	0.11	0.25

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,586)	1:B:275:GLU:HG3	1:B:276:ASN:H	5	0.25	0.1	0.25
(1,910)	1:A:103:ASN:H	1:A:124:ILE:HG21	5	0.24	0.1	0.27
(1,910)	1:A:103:ASN:H	1:A:124:ILE:HG22	5	0.24	0.1	0.27
(1,910)	1:A:103:ASN:H	1:A:124:ILE:HG23	5	0.24	0.1	0.27
(1,1234)	1:B:217:VAL:HG11	1:B:228:PHE:H	5	0.22	0.09	0.19
(1,1234)	1:B:217:VAL:HG12	1:B:228:PHE:H	5	0.22	0.09	0.19
(1,1234)	1:B:217:VAL:HG13	1:B:228:PHE:H	5	0.22	0.09	0.19
(1,897)	1:A:102:ARG:HG2	1:A:103:ASN:H	5	0.21	0.06	0.21
(1,912)	1:B:303:ASN:H	1:B:324:ILE:HG21	5	0.2	0.05	0.2
(1,912)	1:B:303:ASN:H	1:B:324:ILE:HG22	5	0.2	0.05	0.2
(1,912)	1:B:303:ASN:H	1:B:324:ILE:HG23	5	0.2	0.05	0.2
(1,198)	1:A:72:MET:H	1:A:73:PRO:HA	5	0.19	0.03	0.19
(1,1233)	1:A:17:VAL:HG11	1:A:28:PHE:H	5	0.18	0.08	0.15
(1,1233)	1:A:17:VAL:HG12	1:A:28:PHE:H	5	0.18	0.08	0.15
(1,1233)	1:A:17:VAL:HG13	1:A:28:PHE:H	5	0.18	0.08	0.15
(1,55)	1:A:103:ASN:HA	1:A:124:ILE:HA	5	0.17	0.03	0.18
(1,354)	1:B:217:VAL:HG11	1:B:218:TRP:HA	5	0.15	0.02	0.15
(1,354)	1:B:217:VAL:HG12	1:B:218:TRP:HA	5	0.15	0.02	0.15
(1,354)	1:B:217:VAL:HG13	1:B:218:TRP:HA	5	0.15	0.02	0.15
(1,754)	1:B:306:THR:HG21	1:B:323:ALA:H	5	0.14	0.03	0.13
(1,754)	1:B:306:THR:HG22	1:B:323:ALA:H	5	0.14	0.03	0.13
(1,754)	1:B:306:THR:HG23	1:B:323:ALA:H	5	0.14	0.03	0.13
(1,29)	1:A:32:LEU:HD11	1:A:33:LEU:HA	4	1.24	0.24	1.32
(1,29)	1:A:32:LEU:HD12	1:A:33:LEU:HA	4	1.24	0.24	1.32
(1,29)	1:A:32:LEU:HD13	1:A:33:LEU:HA	4	1.24	0.24	1.32
(1,1250)	1:B:270:VAL:HG11	1:B:272:MET:H	4	0.96	0.82	0.72
(1,1250)	1:B:270:VAL:HG12	1:B:272:MET:H	4	0.96	0.82	0.72
(1,1250)	1:B:270:VAL:HG13	1:B:272:MET:H	4	0.96	0.82	0.72
(1,554)	1:B:224:LEU:HB3	1:B:226:THR:HA	4	0.61	0.28	0.64
(1,165)	1:B:247:VAL:HG21	1:B:286:SER:HA	4	0.47	0.21	0.44
(1,165)	1:B:247:VAL:HG22	1:B:286:SER:HA	4	0.47	0.21	0.44
(1,165)	1:B:247:VAL:HG23	1:B:286:SER:HA	4	0.47	0.21	0.44
(1,1225)	1:B:217:VAL:HG11	1:B:229:SER:H	4	0.38	0.15	0.45
(1,1225)	1:B:217:VAL:HG12	1:B:229:SER:H	4	0.38	0.15	0.45
(1,1225)	1:B:217:VAL:HG13	1:B:229:SER:H	4	0.38	0.15	0.45
(1,1223)	1:A:17:VAL:HG11	1:A:29:SER:H	4	0.34	0.15	0.32
(1,1223)	1:A:17:VAL:HG12	1:A:29:SER:H	4	0.34	0.15	0.32
(1,1223)	1:A:17:VAL:HG13	1:A:29:SER:H	4	0.34	0.15	0.32
(1,308)	1:B:302:ARG:HG2	1:B:303:ASN:HA	4	0.31	0.05	0.31
(1,526)	1:A:16:ILE:HB	1:A:29:SER:HA	4	0.29	0.15	0.28
(1,1235)	1:A:18:TRP:HB2	1:A:28:PHE:H	4	0.26	0.06	0.24
(1,1235)	1:A:18:TRP:HB3	1:A:28:PHE:H	4	0.26	0.06	0.24

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,898)	1:B:302:ARG:HG2	1:B:303:ASN:H	4	0.21	0.05	0.2
(1,649)	1:A:114:GLY:HA3	1:A:115:LEU:HG	4	0.17	0.02	0.18
(1,56)	1:B:303:ASN:HA	1:B:324:ILE:HA	4	0.16	0.04	0.16
(1,199)	1:B:259:ALA:H	1:B:273:PRO:HA	4	0.15	0.04	0.14
(1,353)	1:A:17:VAL:HG11	1:A:18:TRP:HA	4	0.14	0.03	0.12
(1,353)	1:A:17:VAL:HG12	1:A:18:TRP:HA	4	0.14	0.03	0.12
(1,353)	1:A:17:VAL:HG13	1:A:18:TRP:HA	4	0.14	0.03	0.12
(1,197)	1:A:59:ALA:H	1:A:73:PRO:HA	4	0.13	0.02	0.12
(1,673)	1:A:87:ALA:HB1	1:A:88:GLU:HB3	4	0.12	0.02	0.11
(1,673)	1:A:87:ALA:HB2	1:A:88:GLU:HB3	4	0.12	0.02	0.11
(1,673)	1:A:87:ALA:HB3	1:A:88:GLU:HB3	4	0.12	0.02	0.11
(1,393)	1:A:124:ILE:HD11	1:A:125:VAL:HG21	3	0.71	0.49	0.64
(1,393)	1:A:124:ILE:HD11	1:A:125:VAL:HG22	3	0.71	0.49	0.64
(1,393)	1:A:124:ILE:HD11	1:A:125:VAL:HG23	3	0.71	0.49	0.64
(1,393)	1:A:124:ILE:HD12	1:A:125:VAL:HG21	3	0.71	0.49	0.64
(1,393)	1:A:124:ILE:HD12	1:A:125:VAL:HG22	3	0.71	0.49	0.64
(1,393)	1:A:124:ILE:HD12	1:A:125:VAL:HG23	3	0.71	0.49	0.64
(1,393)	1:A:124:ILE:HD13	1:A:125:VAL:HG21	3	0.71	0.49	0.64
(1,393)	1:A:124:ILE:HD13	1:A:125:VAL:HG22	3	0.71	0.49	0.64
(1,393)	1:A:124:ILE:HD13	1:A:125:VAL:HG23	3	0.71	0.49	0.64
(1,616)	1:A:102:ARG:HB2	1:A:103:ASN:HB2	3	0.49	0.07	0.53
(1,616)	1:A:102:ARG:HB3	1:A:103:ASN:HB2	3	0.49	0.07	0.53
(1,581)	1:A:44:LEU:HD11	1:B:273:PRO:HB3	3	0.46	0.21	0.39
(1,581)	1:A:44:LEU:HD12	1:B:273:PRO:HB3	3	0.46	0.21	0.39
(1,581)	1:A:44:LEU:HD13	1:B:273:PRO:HB3	3	0.46	0.21	0.39
(1,680)	1:B:293:LEU:HD11	1:B:294:LYS:HG2	3	0.44	0.39	0.17
(1,680)	1:B:293:LEU:HD12	1:B:294:LYS:HG2	3	0.44	0.39	0.17
(1,680)	1:B:293:LEU:HD13	1:B:294:LYS:HG2	3	0.44	0.39	0.17
(1,778)	1:A:32:LEU:HD11	1:B:316:GLY:H	3	0.42	0.28	0.3
(1,778)	1:A:32:LEU:HD12	1:B:316:GLY:H	3	0.42	0.28	0.3
(1,778)	1:A:32:LEU:HD13	1:B:316:GLY:H	3	0.42	0.28	0.3
(1,258)	1:A:28:PHE:HA	1:A:52:VAL:HB	3	0.39	0.18	0.51
(1,206)	1:B:252:VAL:HB	1:B:253:SER:HA	3	0.38	0.01	0.39
(1,376)	1:B:217:VAL:HB	1:B:227:THR:HB	3	0.38	0.1	0.38
(1,163)	1:A:47:VAL:HG21	1:A:86:SER:HA	3	0.33	0.18	0.26
(1,163)	1:A:47:VAL:HG22	1:A:86:SER:HA	3	0.33	0.18	0.26
(1,163)	1:A:47:VAL:HG23	1:A:86:SER:HA	3	0.33	0.18	0.26
(1,259)	1:B:217:VAL:HB	1:B:228:PHE:HA	3	0.33	0.15	0.26
(1,456)	1:A:102:ARG:HB2	1:A:105:ASP:HB2	3	0.33	0.08	0.35
(1,456)	1:A:102:ARG:HB3	1:A:105:ASP:HB2	3	0.33	0.08	0.35
(1,1085)	1:A:78:SER:H	1:A:79:ILE:HG12	3	0.33	0.15	0.24
(1,459)	1:B:302:ARG:HB2	1:B:305:ASP:HB2	3	0.31	0.09	0.32

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,459)	1:B:302:ARG:HB3	1:B:305:ASP:HB2	3	0.31	0.09	0.32
(1,1087)	1:B:278:SER:H	1:B:279:ILE:HG12	3	0.29	0.19	0.19
(1,594)	1:A:49:GLY:H	1:A:50:GLN:HB2	3	0.25	0.06	0.25
(1,377)	1:A:17:VAL:HG11	1:A:27:THR:HB	3	0.22	0.03	0.21
(1,377)	1:A:17:VAL:HG12	1:A:27:THR:HB	3	0.22	0.03	0.21
(1,377)	1:A:17:VAL:HG13	1:A:27:THR:HB	3	0.22	0.03	0.21
(1,1153)	1:A:50:GLN:H	1:A:50:GLN:HG2	3	0.21	0.09	0.17
(1,1153)	1:A:50:GLN:H	1:A:50:GLN:HG3	3	0.21	0.09	0.17
(1,1155)	1:B:250:GLN:H	1:B:250:GLN:HG2	3	0.2	0.07	0.18
(1,1155)	1:B:250:GLN:H	1:B:250:GLN:HG3	3	0.2	0.07	0.18
(1,690)	1:B:208:PRO:HG2	1:B:218:TRP:HB2	3	0.19	0.06	0.21
(1,690)	1:B:208:PRO:HG2	1:B:218:TRP:HB3	3	0.19	0.06	0.21
(1,690)	1:B:208:PRO:HG3	1:B:218:TRP:HB2	3	0.19	0.06	0.21
(1,690)	1:B:208:PRO:HG3	1:B:218:TRP:HB3	3	0.19	0.06	0.21
(1,851)	1:A:97:TRP:HE1	1:B:305:ASP:H	3	0.16	0.04	0.14
(1,375)	1:A:17:VAL:HB	1:A:27:THR:HB	3	0.15	0.02	0.15
(1,319)	1:B:275:GLU:HA	1:B:276:ASN:HB3	3	0.15	0.02	0.15
(1,674)	1:B:287:ALA:HB1	1:B:288:GLU:HB3	3	0.14	0.02	0.14
(1,674)	1:B:287:ALA:HB2	1:B:288:GLU:HB3	3	0.14	0.02	0.14
(1,674)	1:B:287:ALA:HB3	1:B:288:GLU:HB3	3	0.14	0.02	0.14
(1,1141)	1:A:50:GLN:H	1:A:83:ILE:H	3	0.14	0.04	0.11
(1,216)	1:B:251:TYR:HA	1:B:252:VAL:HB	3	0.14	0.02	0.13
(1,1034)	1:A:79:ILE:HD11	1:B:284:SER:H	3	0.13	0.03	0.12
(1,1034)	1:A:79:ILE:HD12	1:B:284:SER:H	3	0.13	0.03	0.12
(1,1034)	1:A:79:ILE:HD13	1:B:284:SER:H	3	0.13	0.03	0.12
(1,1142)	1:B:250:GLN:H	1:B:283:ILE:H	3	0.13	0.02	0.12
(1,125)	1:A:93:LEU:HA	1:A:97:TRP:HA	3	0.13	0.01	0.13
(1,174)	1:B:248:SER:HA	1:B:283:ILE:HA	3	0.12	0.0	0.12
(1,1162)	1:B:293:LEU:H	1:B:296:GLU:H	3	0.11	0.0	0.11
(1,613)	1:A:20:ASP:HA	1:A:23:ARG:HB2	2	1.42	0.41	1.42
(1,523)	1:A:125:VAL:HB	1:A:126:SER:HA	2	1.07	0.02	1.07
(1,584)	1:A:75:GLU:HB3	1:B:244:LEU:HD11	2	0.82	0.18	0.82
(1,584)	1:A:75:GLU:HB3	1:B:244:LEU:HD12	2	0.82	0.18	0.82
(1,584)	1:A:75:GLU:HB3	1:B:244:LEU:HD13	2	0.82	0.18	0.82
(1,579)	1:A:125:VAL:HG11	1:B:205:PRO:HB2	2	0.74	0.04	0.74
(1,579)	1:A:125:VAL:HG12	1:B:205:PRO:HB2	2	0.74	0.04	0.74
(1,579)	1:A:125:VAL:HG13	1:B:205:PRO:HB2	2	0.74	0.04	0.74
(1,582)	1:A:44:LEU:HD11	1:B:275:GLU:HB3	2	0.7	0.14	0.7
(1,582)	1:A:44:LEU:HD12	1:B:275:GLU:HB3	2	0.7	0.14	0.7
(1,582)	1:A:44:LEU:HD13	1:B:275:GLU:HB3	2	0.7	0.14	0.7
(1,64)	1:B:307:LEU:HD11	1:B:308:PHE:HA	2	0.69	0.06	0.69
(1,64)	1:B:307:LEU:HD12	1:B:308:PHE:HA	2	0.69	0.06	0.69

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,64)	1:B:307:LEU:HD13	1:B:308:PHE:HA	2	0.69	0.06	0.69
(1,63)	1:A:107:LEU:HD11	1:A:108:PHE:HA	2	0.68	0.09	0.68
(1,63)	1:A:107:LEU:HD12	1:A:108:PHE:HA	2	0.68	0.09	0.68
(1,63)	1:A:107:LEU:HD13	1:A:108:PHE:HA	2	0.68	0.09	0.68
(1,583)	1:A:73:PRO:HB3	1:B:244:LEU:HD11	2	0.64	0.18	0.64
(1,583)	1:A:73:PRO:HB3	1:B:244:LEU:HD12	2	0.64	0.18	0.64
(1,583)	1:A:73:PRO:HB3	1:B:244:LEU:HD13	2	0.64	0.18	0.64
(1,718)	1:B:302:ARG:HG2	1:B:325:VAL:H	2	0.62	0.36	0.62
(1,515)	1:A:125:VAL:HB	1:A:126:SER:HB2	2	0.45	0.03	0.45
(1,515)	1:A:125:VAL:HB	1:A:126:SER:HB3	2	0.45	0.03	0.45
(1,641)	1:A:53:SER:H	1:A:54:VAL:HG21	2	0.41	0.02	0.41
(1,641)	1:A:53:SER:H	1:A:54:VAL:HG22	2	0.41	0.02	0.41
(1,641)	1:A:53:SER:H	1:A:54:VAL:HG23	2	0.41	0.02	0.41
(1,720)	1:A:103:ASN:HB3	1:A:125:VAL:H	2	0.4	0.0	0.4
(1,98)	1:B:270:VAL:HG11	1:B:271:ILE:HA	2	0.35	0.19	0.35
(1,98)	1:B:270:VAL:HG12	1:B:271:ILE:HA	2	0.35	0.19	0.35
(1,98)	1:B:270:VAL:HG13	1:B:271:ILE:HA	2	0.35	0.19	0.35
(1,723)	1:B:303:ASN:HB3	1:B:325:VAL:H	2	0.34	0.06	0.34
(1,507)	1:A:54:VAL:HB	1:A:78:SER:HA	2	0.32	0.2	0.32
(1,642)	1:B:253:SER:H	1:B:254:VAL:HG21	2	0.32	0.06	0.32
(1,642)	1:B:253:SER:H	1:B:254:VAL:HG22	2	0.32	0.06	0.32
(1,642)	1:B:253:SER:H	1:B:254:VAL:HG23	2	0.32	0.06	0.32
(1,506)	1:B:254:VAL:HB	1:B:255:TYR:HA	2	0.29	0.1	0.29
(1,394)	1:B:324:ILE:HD11	1:B:325:VAL:HG21	2	0.29	0.14	0.29
(1,394)	1:B:324:ILE:HD11	1:B:325:VAL:HG22	2	0.29	0.14	0.29
(1,394)	1:B:324:ILE:HD11	1:B:325:VAL:HG23	2	0.29	0.14	0.29
(1,394)	1:B:324:ILE:HD12	1:B:325:VAL:HG21	2	0.29	0.14	0.29
(1,394)	1:B:324:ILE:HD12	1:B:325:VAL:HG22	2	0.29	0.14	0.29
(1,394)	1:B:324:ILE:HD12	1:B:325:VAL:HG23	2	0.29	0.14	0.29
(1,394)	1:B:324:ILE:HD13	1:B:325:VAL:HG21	2	0.29	0.14	0.29
(1,394)	1:B:324:ILE:HD13	1:B:325:VAL:HG22	2	0.29	0.14	0.29
(1,394)	1:B:324:ILE:HD13	1:B:325:VAL:HG23	2	0.29	0.14	0.29
(1,959)	1:A:92:THR:HG21	1:A:95:ALA:H	2	0.29	0.14	0.29
(1,959)	1:A:92:THR:HG22	1:A:95:ALA:H	2	0.29	0.14	0.29
(1,959)	1:A:92:THR:HG23	1:A:95:ALA:H	2	0.29	0.14	0.29
(1,306)	1:B:231:SER:HA	1:B:250:GLN:H	2	0.24	0.08	0.24
(1,106)	1:B:295:ALA:HA	1:B:296:GLU:HG2	2	0.24	0.11	0.24
(1,106)	1:B:295:ALA:HA	1:B:296:GLU:HG3	2	0.24	0.11	0.24
(1,1269)	1:A:115:LEU:H	1:A:117:PHE:H	2	0.22	0.1	0.22
(1,504)	1:A:54:VAL:HB	1:A:55:TYR:HA	2	0.22	0.02	0.22
(1,1036)	1:A:84:SER:H	1:B:279:ILE:HD11	2	0.22	0.02	0.22
(1,1036)	1:A:84:SER:H	1:B:279:ILE:HD12	2	0.22	0.02	0.22

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1036)	1:A:84:SER:H	1:B:279:ILE:HD13	2	0.22	0.02	0.22
(1,359)	1:A:16:ILE:HA	1:A:17:VAL:HG11	2	0.2	0.06	0.2
(1,359)	1:A:16:ILE:HA	1:A:17:VAL:HG12	2	0.2	0.06	0.2
(1,359)	1:A:16:ILE:HA	1:A:17:VAL:HG13	2	0.2	0.06	0.2
(1,503)	1:A:28:PHE:HA	1:A:54:VAL:HB	2	0.2	0.06	0.2
(1,172)	1:A:48:SER:HA	1:A:83:ILE:HA	2	0.2	0.01	0.2
(1,361)	1:B:216:ILE:HA	1:B:217:VAL:HG11	2	0.2	0.04	0.2
(1,361)	1:B:216:ILE:HA	1:B:217:VAL:HG12	2	0.2	0.04	0.2
(1,361)	1:B:216:ILE:HA	1:B:217:VAL:HG13	2	0.2	0.04	0.2
(1,650)	1:B:314:GLY:HA3	1:B:315:LEU:HG	2	0.2	0.02	0.2
(1,931)	1:B:232:LEU:HD11	1:B:233:LEU:H	2	0.18	0.07	0.18
(1,931)	1:B:232:LEU:HD12	1:B:233:LEU:H	2	0.18	0.07	0.18
(1,931)	1:B:232:LEU:HD13	1:B:233:LEU:H	2	0.18	0.07	0.18
(1,1296)	1:A:97:TRP:HE1	1:B:305:ASP:HA	2	0.18	0.04	0.18
(1,317)	1:A:75:GLU:HA	1:A:76:ASN:HB3	2	0.16	0.03	0.16
(1,380)	1:B:227:THR:HB	1:B:254:VAL:HG21	2	0.16	0.03	0.16
(1,380)	1:B:227:THR:HB	1:B:254:VAL:HG22	2	0.16	0.03	0.16
(1,380)	1:B:227:THR:HB	1:B:254:VAL:HG23	2	0.16	0.03	0.16
(1,678)	1:A:93:LEU:HD11	1:A:94:LYS:HG2	2	0.16	0.01	0.16
(1,678)	1:A:93:LEU:HD12	1:A:94:LYS:HG2	2	0.16	0.01	0.16
(1,678)	1:A:93:LEU:HD13	1:A:94:LYS:HG2	2	0.16	0.01	0.16
(1,1161)	1:A:93:LEU:H	1:A:96:GLU:H	2	0.16	0.01	0.16
(1,438)	1:A:69:CYS:HA	1:A:70:VAL:HG11	2	0.16	0.05	0.16
(1,438)	1:A:69:CYS:HA	1:A:70:VAL:HG12	2	0.16	0.05	0.16
(1,438)	1:A:69:CYS:HA	1:A:70:VAL:HG13	2	0.16	0.05	0.16
(1,100)	1:B:294:LYS:HA	1:B:297:TRP:HA	2	0.15	0.02	0.15
(1,1160)	1:B:250:GLN:H	1:B:250:GLN:HB2	2	0.15	0.01	0.15
(1,111)	1:A:95:ALA:HA	1:A:98:GLU:HB3	2	0.14	0.01	0.14
(1,112)	1:B:295:ALA:HA	1:B:298:GLU:HB3	2	0.14	0.01	0.14
(1,128)	1:B:293:LEU:HA	1:B:297:TRP:HA	2	0.14	0.01	0.14
(1,352)	1:B:208:PRO:HA	1:B:218:TRP:HA	2	0.14	0.03	0.14
(1,919)	1:A:101:LYS:H	1:A:102:ARG:HB2	2	0.14	0.02	0.14
(1,919)	1:A:101:LYS:H	1:A:102:ARG:HB3	2	0.14	0.02	0.14
(1,1219)	1:A:17:VAL:HA	1:A:30:ALA:H	2	0.14	0.01	0.14
(1,1270)	1:B:315:LEU:H	1:B:317:PHE:H	2	0.14	0.02	0.14
(1,1194)	1:B:241:ILE:HB	1:B:242:ALA:H	2	0.14	0.02	0.14
(1,1295)	1:A:105:ASP:HA	1:B:297:TRP:HE1	2	0.14	0.01	0.14
(1,1078)	1:A:80:ARG:H	1:B:282:VAL:HG11	2	0.13	0.01	0.13
(1,1078)	1:A:80:ARG:H	1:B:282:VAL:HG12	2	0.13	0.01	0.13
(1,1078)	1:A:80:ARG:H	1:B:282:VAL:HG13	2	0.13	0.01	0.13
(1,31)	1:A:112:ASN:HA	1:A:115:LEU:H	2	0.12	0.01	0.12
(1,105)	1:A:95:ALA:HA	1:A:96:GLU:HG2	2	0.12	0.01	0.12

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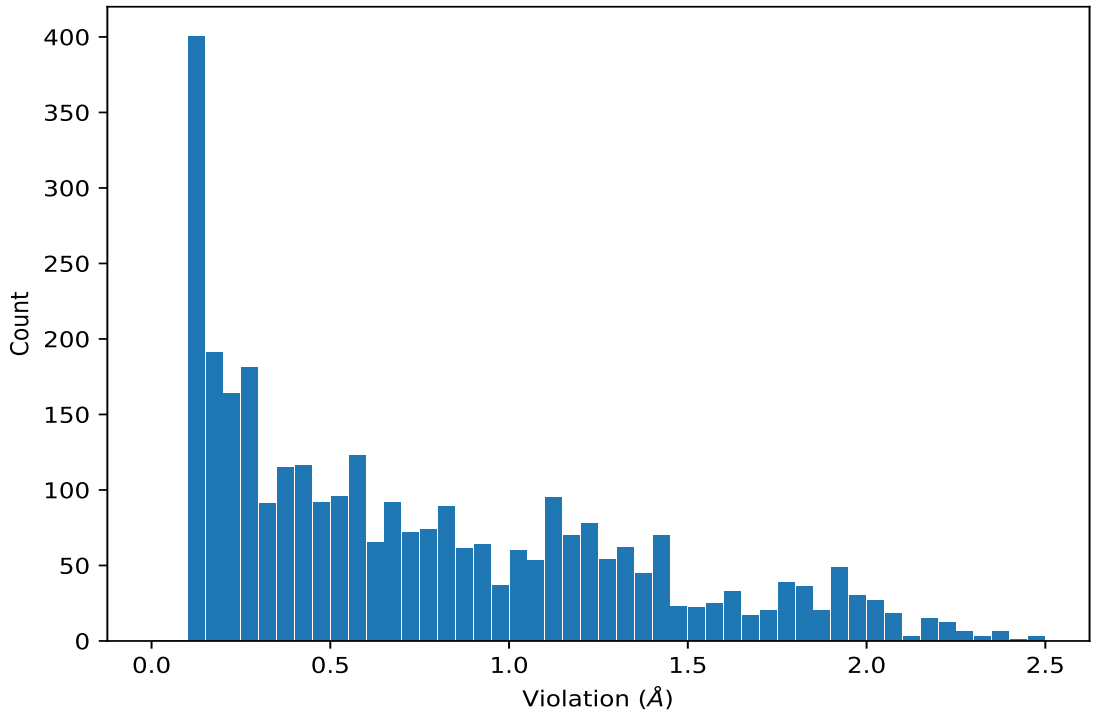
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,105)	1:A:95:ALA:HA	1:A:96:GLU:HG3	2	0.12	0.01	0.12

[1]Number of violated models, [2]Standard deviation

9.5 All violated distance restraints

9.5.1 Histogram : Distribution of distance violations

The following histogram shows the distribution of the absolute value of the violation for all violated restraints in the ensemble.



9.5.2 Table : All distance violations

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,34)	1:B:312:ASN:HA	1:B:315:LEU:HD21	13	2.48
(1,34)	1:B:312:ASN:HA	1:B:315:LEU:HD22	13	2.48
(1,34)	1:B:312:ASN:HA	1:B:315:LEU:HD23	13	2.48

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,498)	1:B:220:ASP:HB2	1:B:223:ARG:HD3	16	2.44
(1,679)	1:B:290:LEU:HD11	1:B:294:LYS:HG2	2	2.39
(1,679)	1:B:290:LEU:HD12	1:B:294:LYS:HG2	2	2.39
(1,679)	1:B:290:LEU:HD13	1:B:294:LYS:HG2	2	2.39
(1,677)	1:A:90:LEU:HD11	1:A:94:LYS:HG2	2	2.39
(1,677)	1:A:90:LEU:HD12	1:A:94:LYS:HG2	2	2.39
(1,677)	1:A:90:LEU:HD13	1:A:94:LYS:HG2	2	2.39
(1,1250)	1:B:270:VAL:HG11	1:B:272:MET:H	10	2.32
(1,1250)	1:B:270:VAL:HG12	1:B:272:MET:H	10	2.32
(1,1250)	1:B:270:VAL:HG13	1:B:272:MET:H	10	2.32
(1,1312)	1:B:232:LEU:HD11	1:B:234:ARG:H	7	2.29
(1,1312)	1:B:232:LEU:HD12	1:B:234:ARG:H	7	2.29
(1,1312)	1:B:232:LEU:HD13	1:B:234:ARG:H	7	2.29
(1,1249)	1:A:70:VAL:HG11	1:A:72:MET:H	20	2.28
(1,1249)	1:A:70:VAL:HG12	1:A:72:MET:H	20	2.28
(1,1249)	1:A:70:VAL:HG13	1:A:72:MET:H	20	2.28
(1,34)	1:B:312:ASN:HA	1:B:315:LEU:HD21	15	2.2
(1,34)	1:B:312:ASN:HA	1:B:315:LEU:HD22	15	2.2
(1,34)	1:B:312:ASN:HA	1:B:315:LEU:HD23	15	2.2
(1,34)	1:B:312:ASN:HA	1:B:315:LEU:HD21	18	2.2
(1,34)	1:B:312:ASN:HA	1:B:315:LEU:HD22	18	2.2
(1,34)	1:B:312:ASN:HA	1:B:315:LEU:HD23	18	2.2
(1,33)	1:A:112:ASN:HA	1:A:115:LEU:HD21	14	2.2
(1,33)	1:A:112:ASN:HA	1:A:115:LEU:HD22	14	2.2
(1,33)	1:A:112:ASN:HA	1:A:115:LEU:HD23	14	2.2
(1,33)	1:A:112:ASN:HA	1:A:115:LEU:HD21	18	2.2
(1,33)	1:A:112:ASN:HA	1:A:115:LEU:HD22	18	2.2
(1,33)	1:A:112:ASN:HA	1:A:115:LEU:HD23	18	2.2
(1,33)	1:A:112:ASN:HA	1:A:115:LEU:HD21	15	2.19
(1,33)	1:A:112:ASN:HA	1:A:115:LEU:HD22	15	2.19
(1,33)	1:A:112:ASN:HA	1:A:115:LEU:HD23	15	2.19
(1,34)	1:B:312:ASN:HA	1:B:315:LEU:HD21	14	2.17
(1,34)	1:B:312:ASN:HA	1:B:315:LEU:HD22	14	2.17
(1,34)	1:B:312:ASN:HA	1:B:315:LEU:HD23	14	2.17
(1,33)	1:A:112:ASN:HA	1:A:115:LEU:HD21	12	2.17
(1,33)	1:A:112:ASN:HA	1:A:115:LEU:HD22	12	2.17
(1,33)	1:A:112:ASN:HA	1:A:115:LEU:HD23	12	2.17
(1,679)	1:B:290:LEU:HD11	1:B:294:LYS:HG2	3	2.16
(1,679)	1:B:290:LEU:HD12	1:B:294:LYS:HG2	3	2.16
(1,679)	1:B:290:LEU:HD13	1:B:294:LYS:HG2	3	2.16
(1,1267)	1:A:17:VAL:HG11	1:A:19:SER:H	17	2.15
(1,1267)	1:A:17:VAL:HG12	1:A:19:SER:H	17	2.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1267)	1:A:17:VAL:HG13	1:A:19:SER:H	17	2.15
(1,677)	1:A:90:LEU:HD11	1:A:94:LYS:HG2	3	2.13
(1,677)	1:A:90:LEU:HD12	1:A:94:LYS:HG2	3	2.13
(1,677)	1:A:90:LEU:HD13	1:A:94:LYS:HG2	3	2.13
(1,628)	1:A:52:VAL:HG21	1:A:79:ILE:HA	12	2.09
(1,628)	1:A:52:VAL:HG22	1:A:79:ILE:HA	12	2.09
(1,628)	1:A:52:VAL:HG23	1:A:79:ILE:HA	12	2.09
(1,627)	1:A:52:VAL:HG21	1:A:54:VAL:HA	18	2.09
(1,627)	1:A:52:VAL:HG22	1:A:54:VAL:HA	18	2.09
(1,627)	1:A:52:VAL:HG23	1:A:54:VAL:HA	18	2.09
(1,1268)	1:B:217:VAL:HG11	1:B:219:SER:H	9	2.08
(1,1268)	1:B:217:VAL:HG12	1:B:219:SER:H	9	2.08
(1,1268)	1:B:217:VAL:HG13	1:B:219:SER:H	9	2.08
(1,800)	1:B:312:ASN:H	1:B:315:LEU:HD21	18	2.07
(1,800)	1:B:312:ASN:H	1:B:315:LEU:HD22	18	2.07
(1,800)	1:B:312:ASN:H	1:B:315:LEU:HD23	18	2.07
(1,799)	1:A:112:ASN:H	1:A:115:LEU:HD21	18	2.07
(1,799)	1:A:112:ASN:H	1:A:115:LEU:HD22	18	2.07
(1,799)	1:A:112:ASN:H	1:A:115:LEU:HD23	18	2.07
(1,1267)	1:A:17:VAL:HG11	1:A:19:SER:H	14	2.06
(1,1267)	1:A:17:VAL:HG12	1:A:19:SER:H	14	2.06
(1,1267)	1:A:17:VAL:HG13	1:A:19:SER:H	14	2.06
(1,629)	1:B:252:VAL:HG21	1:B:254:VAL:HA	11	2.05
(1,629)	1:B:252:VAL:HG22	1:B:254:VAL:HA	11	2.05
(1,629)	1:B:252:VAL:HG23	1:B:254:VAL:HA	11	2.05
(1,1267)	1:A:17:VAL:HG11	1:A:19:SER:H	1	2.04
(1,1267)	1:A:17:VAL:HG12	1:A:19:SER:H	1	2.04
(1,1267)	1:A:17:VAL:HG13	1:A:19:SER:H	1	2.04
(1,1267)	1:A:17:VAL:HG11	1:A:19:SER:H	4	2.04
(1,1267)	1:A:17:VAL:HG12	1:A:19:SER:H	4	2.04
(1,1267)	1:A:17:VAL:HG13	1:A:19:SER:H	4	2.04
(1,800)	1:B:312:ASN:H	1:B:315:LEU:HD21	13	2.03
(1,800)	1:B:312:ASN:H	1:B:315:LEU:HD22	13	2.03
(1,800)	1:B:312:ASN:H	1:B:315:LEU:HD23	13	2.03
(1,629)	1:B:252:VAL:HG21	1:B:254:VAL:HA	20	2.03
(1,629)	1:B:252:VAL:HG22	1:B:254:VAL:HA	20	2.03
(1,629)	1:B:252:VAL:HG23	1:B:254:VAL:HA	20	2.03
(1,1214)	1:A:31:SER:H	1:A:52:VAL:HG11	16	2.02
(1,1214)	1:A:31:SER:H	1:A:52:VAL:HG12	16	2.02
(1,1214)	1:A:31:SER:H	1:A:52:VAL:HG13	16	2.02
(1,627)	1:A:52:VAL:HG21	1:A:54:VAL:HA	14	2.01
(1,627)	1:A:52:VAL:HG22	1:A:54:VAL:HA	14	2.01

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,627)	1:A:52:VAL:HG23	1:A:54:VAL:HA	14	2.01
(1,627)	1:A:52:VAL:HG21	1:A:54:VAL:HA	17	2.0
(1,627)	1:A:52:VAL:HG22	1:A:54:VAL:HA	17	2.0
(1,627)	1:A:52:VAL:HG23	1:A:54:VAL:HA	17	2.0
(1,34)	1:B:312:ASN:HA	1:B:315:LEU:HD21	12	2.0
(1,34)	1:B:312:ASN:HA	1:B:315:LEU:HD22	12	2.0
(1,34)	1:B:312:ASN:HA	1:B:315:LEU:HD23	12	2.0
(1,629)	1:B:252:VAL:HG21	1:B:254:VAL:HA	17	1.99
(1,629)	1:B:252:VAL:HG22	1:B:254:VAL:HA	17	1.99
(1,629)	1:B:252:VAL:HG23	1:B:254:VAL:HA	17	1.99
(1,1268)	1:B:217:VAL:HG11	1:B:219:SER:H	15	1.98
(1,1268)	1:B:217:VAL:HG12	1:B:219:SER:H	15	1.98
(1,1268)	1:B:217:VAL:HG13	1:B:219:SER:H	15	1.98
(1,1267)	1:A:17:VAL:HG11	1:A:19:SER:H	11	1.98
(1,1267)	1:A:17:VAL:HG12	1:A:19:SER:H	11	1.98
(1,1267)	1:A:17:VAL:HG13	1:A:19:SER:H	11	1.98
(1,629)	1:B:252:VAL:HG21	1:B:254:VAL:HA	9	1.97
(1,629)	1:B:252:VAL:HG22	1:B:254:VAL:HA	9	1.97
(1,629)	1:B:252:VAL:HG23	1:B:254:VAL:HA	9	1.97
(1,627)	1:A:52:VAL:HG21	1:A:54:VAL:HA	10	1.97
(1,627)	1:A:52:VAL:HG22	1:A:54:VAL:HA	10	1.97
(1,627)	1:A:52:VAL:HG23	1:A:54:VAL:HA	10	1.97
(1,627)	1:A:52:VAL:HG21	1:A:54:VAL:HA	20	1.97
(1,627)	1:A:52:VAL:HG22	1:A:54:VAL:HA	20	1.97
(1,627)	1:A:52:VAL:HG23	1:A:54:VAL:HA	20	1.97
(1,629)	1:B:252:VAL:HG21	1:B:254:VAL:HA	5	1.96
(1,629)	1:B:252:VAL:HG22	1:B:254:VAL:HA	5	1.96
(1,629)	1:B:252:VAL:HG23	1:B:254:VAL:HA	5	1.96
(1,627)	1:A:52:VAL:HG21	1:A:54:VAL:HA	11	1.96
(1,627)	1:A:52:VAL:HG22	1:A:54:VAL:HA	11	1.96
(1,627)	1:A:52:VAL:HG23	1:A:54:VAL:HA	11	1.96
(1,1268)	1:B:217:VAL:HG11	1:B:219:SER:H	5	1.96
(1,1268)	1:B:217:VAL:HG12	1:B:219:SER:H	5	1.96
(1,1268)	1:B:217:VAL:HG13	1:B:219:SER:H	5	1.96
(1,1267)	1:A:17:VAL:HG11	1:A:19:SER:H	5	1.96
(1,1267)	1:A:17:VAL:HG12	1:A:19:SER:H	5	1.96
(1,1267)	1:A:17:VAL:HG13	1:A:19:SER:H	5	1.96
(1,629)	1:B:252:VAL:HG21	1:B:254:VAL:HA	13	1.95
(1,629)	1:B:252:VAL:HG22	1:B:254:VAL:HA	13	1.95
(1,629)	1:B:252:VAL:HG23	1:B:254:VAL:HA	13	1.95
(1,1216)	1:B:231:SER:H	1:B:252:VAL:HG11	16	1.95
(1,1216)	1:B:231:SER:H	1:B:252:VAL:HG12	16	1.95

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1216)	1:B:231:SER:H	1:B:252:VAL:HG13	16	1.95
(1,1214)	1:A:31:SER:H	1:A:52:VAL:HG11	15	1.95
(1,1214)	1:A:31:SER:H	1:A:52:VAL:HG12	15	1.95
(1,1214)	1:A:31:SER:H	1:A:52:VAL:HG13	15	1.95
(1,102)	1:B:293:LEU:HD11	1:B:297:TRP:HA	12	1.95
(1,102)	1:B:293:LEU:HD12	1:B:297:TRP:HA	12	1.95
(1,102)	1:B:293:LEU:HD13	1:B:297:TRP:HA	12	1.95
(1,629)	1:B:252:VAL:HG21	1:B:254:VAL:HA	10	1.94
(1,629)	1:B:252:VAL:HG22	1:B:254:VAL:HA	10	1.94
(1,629)	1:B:252:VAL:HG23	1:B:254:VAL:HA	10	1.94
(1,1214)	1:A:31:SER:H	1:A:52:VAL:HG11	7	1.94
(1,1214)	1:A:31:SER:H	1:A:52:VAL:HG12	7	1.94
(1,1214)	1:A:31:SER:H	1:A:52:VAL:HG13	7	1.94
(1,1214)	1:A:31:SER:H	1:A:52:VAL:HG11	10	1.94
(1,1214)	1:A:31:SER:H	1:A:52:VAL:HG12	10	1.94
(1,1214)	1:A:31:SER:H	1:A:52:VAL:HG13	10	1.94
(1,101)	1:A:93:LEU:HD11	1:A:97:TRP:HA	6	1.94
(1,101)	1:A:93:LEU:HD12	1:A:97:TRP:HA	6	1.94
(1,101)	1:A:93:LEU:HD13	1:A:97:TRP:HA	6	1.94
(1,627)	1:A:52:VAL:HG21	1:A:54:VAL:HA	5	1.93
(1,627)	1:A:52:VAL:HG22	1:A:54:VAL:HA	5	1.93
(1,627)	1:A:52:VAL:HG23	1:A:54:VAL:HA	5	1.93
(1,497)	1:A:20:ASP:HB2	1:A:23:ARG:HD3	20	1.93
(1,95)	1:A:32:LEU:HD11	1:A:34:ARG:HA	11	1.92
(1,95)	1:A:32:LEU:HD12	1:A:34:ARG:HA	11	1.92
(1,95)	1:A:32:LEU:HD13	1:A:34:ARG:HA	11	1.92
(1,1268)	1:B:217:VAL:HG11	1:B:219:SER:H	10	1.92
(1,1268)	1:B:217:VAL:HG12	1:B:219:SER:H	10	1.92
(1,1268)	1:B:217:VAL:HG13	1:B:219:SER:H	10	1.92
(1,1216)	1:B:231:SER:H	1:B:252:VAL:HG11	2	1.92
(1,1216)	1:B:231:SER:H	1:B:252:VAL:HG12	2	1.92
(1,1216)	1:B:231:SER:H	1:B:252:VAL:HG13	2	1.92
(1,1214)	1:A:31:SER:H	1:A:52:VAL:HG11	2	1.92
(1,1214)	1:A:31:SER:H	1:A:52:VAL:HG12	2	1.92
(1,1214)	1:A:31:SER:H	1:A:52:VAL:HG13	2	1.92
(1,101)	1:A:93:LEU:HD11	1:A:97:TRP:HA	12	1.92
(1,101)	1:A:93:LEU:HD12	1:A:97:TRP:HA	12	1.92
(1,101)	1:A:93:LEU:HD13	1:A:97:TRP:HA	12	1.92
(1,1216)	1:B:231:SER:H	1:B:252:VAL:HG11	8	1.91
(1,1216)	1:B:231:SER:H	1:B:252:VAL:HG12	8	1.91
(1,1216)	1:B:231:SER:H	1:B:252:VAL:HG13	8	1.91
(1,1214)	1:A:31:SER:H	1:A:52:VAL:HG11	4	1.91

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1214)	1:A:31:SER:H	1:A:52:VAL:HG12	4	1.91
(1,1214)	1:A:31:SER:H	1:A:52:VAL:HG13	4	1.91
(1,610)	1:B:249:GLY:HA3	1:B:250:GLN:HB2	16	1.89
(1,609)	1:A:49:GLY:HA3	1:A:50:GLN:HB2	4	1.89
(1,1216)	1:B:231:SER:H	1:B:252:VAL:HG11	5	1.87
(1,1216)	1:B:231:SER:H	1:B:252:VAL:HG12	5	1.87
(1,1216)	1:B:231:SER:H	1:B:252:VAL:HG13	5	1.87
(1,630)	1:B:252:VAL:HG21	1:B:279:ILE:HA	20	1.86
(1,630)	1:B:252:VAL:HG22	1:B:279:ILE:HA	20	1.86
(1,630)	1:B:252:VAL:HG23	1:B:279:ILE:HA	20	1.86
(1,628)	1:A:52:VAL:HG21	1:A:79:ILE:HA	20	1.86
(1,628)	1:A:52:VAL:HG22	1:A:79:ILE:HA	20	1.86
(1,628)	1:A:52:VAL:HG23	1:A:79:ILE:HA	20	1.86
(1,610)	1:B:249:GLY:HA3	1:B:250:GLN:HB2	14	1.86
(1,498)	1:B:220:ASP:HB2	1:B:223:ARG:HD3	20	1.86
(1,97)	1:B:232:LEU:HD11	1:B:234:ARG:HA	19	1.85
(1,97)	1:B:232:LEU:HD12	1:B:234:ARG:HA	19	1.85
(1,97)	1:B:232:LEU:HD13	1:B:234:ARG:HA	19	1.85
(1,609)	1:A:49:GLY:HA3	1:A:50:GLN:HB2	5	1.85
(1,1214)	1:A:31:SER:H	1:A:52:VAL:HG11	5	1.85
(1,1214)	1:A:31:SER:H	1:A:52:VAL:HG12	5	1.85
(1,1214)	1:A:31:SER:H	1:A:52:VAL:HG13	5	1.85
(1,679)	1:B:290:LEU:HD11	1:B:294:LYS:HG2	17	1.84
(1,679)	1:B:290:LEU:HD12	1:B:294:LYS:HG2	17	1.84
(1,679)	1:B:290:LEU:HD13	1:B:294:LYS:HG2	17	1.84
(1,629)	1:B:252:VAL:HG21	1:B:254:VAL:HA	1	1.84
(1,629)	1:B:252:VAL:HG22	1:B:254:VAL:HA	1	1.84
(1,629)	1:B:252:VAL:HG23	1:B:254:VAL:HA	1	1.84
(1,627)	1:A:52:VAL:HG21	1:A:54:VAL:HA	9	1.84
(1,627)	1:A:52:VAL:HG22	1:A:54:VAL:HA	9	1.84
(1,627)	1:A:52:VAL:HG23	1:A:54:VAL:HA	9	1.84
(1,1268)	1:B:217:VAL:HG11	1:B:219:SER:H	13	1.84
(1,1268)	1:B:217:VAL:HG12	1:B:219:SER:H	13	1.84
(1,1268)	1:B:217:VAL:HG13	1:B:219:SER:H	13	1.84
(1,677)	1:A:90:LEU:HD11	1:A:94:LYS:HG2	17	1.83
(1,677)	1:A:90:LEU:HD12	1:A:94:LYS:HG2	17	1.83
(1,677)	1:A:90:LEU:HD13	1:A:94:LYS:HG2	17	1.83
(1,627)	1:A:52:VAL:HG21	1:A:54:VAL:HA	2	1.83
(1,627)	1:A:52:VAL:HG22	1:A:54:VAL:HA	2	1.83
(1,627)	1:A:52:VAL:HG23	1:A:54:VAL:HA	2	1.83
(1,613)	1:A:20:ASP:HA	1:A:23:ARG:HB2	17	1.83
(1,609)	1:A:49:GLY:HA3	1:A:50:GLN:HB2	13	1.82

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1214)	1:A:31:SER:H	1:A:52:VAL:HG11	6	1.82
(1,1214)	1:A:31:SER:H	1:A:52:VAL:HG12	6	1.82
(1,1214)	1:A:31:SER:H	1:A:52:VAL:HG13	6	1.82
(1,629)	1:B:252:VAL:HG21	1:B:254:VAL:HA	2	1.81
(1,629)	1:B:252:VAL:HG22	1:B:254:VAL:HA	2	1.81
(1,629)	1:B:252:VAL:HG23	1:B:254:VAL:HA	2	1.81
(1,1268)	1:B:217:VAL:HG11	1:B:219:SER:H	19	1.81
(1,1268)	1:B:217:VAL:HG12	1:B:219:SER:H	19	1.81
(1,1268)	1:B:217:VAL:HG13	1:B:219:SER:H	19	1.81
(1,102)	1:B:293:LEU:HD11	1:B:297:TRP:HA	11	1.81
(1,102)	1:B:293:LEU:HD12	1:B:297:TRP:HA	11	1.81
(1,102)	1:B:293:LEU:HD13	1:B:297:TRP:HA	11	1.81
(1,610)	1:B:249:GLY:HA3	1:B:250:GLN:HB2	13	1.8
(1,33)	1:A:112:ASN:HA	1:A:115:LEU:HD21	4	1.8
(1,33)	1:A:112:ASN:HA	1:A:115:LEU:HD22	4	1.8
(1,33)	1:A:112:ASN:HA	1:A:115:LEU:HD23	4	1.8
(1,677)	1:A:90:LEU:HD11	1:A:94:LYS:HG2	19	1.79
(1,677)	1:A:90:LEU:HD12	1:A:94:LYS:HG2	19	1.79
(1,677)	1:A:90:LEU:HD13	1:A:94:LYS:HG2	19	1.79
(1,627)	1:A:52:VAL:HG21	1:A:54:VAL:HA	12	1.79
(1,627)	1:A:52:VAL:HG22	1:A:54:VAL:HA	12	1.79
(1,627)	1:A:52:VAL:HG23	1:A:54:VAL:HA	12	1.79
(1,1214)	1:A:31:SER:H	1:A:52:VAL:HG11	12	1.79
(1,1214)	1:A:31:SER:H	1:A:52:VAL:HG12	12	1.79
(1,1214)	1:A:31:SER:H	1:A:52:VAL:HG13	12	1.79
(1,679)	1:B:290:LEU:HD11	1:B:294:LYS:HG2	19	1.78
(1,679)	1:B:290:LEU:HD12	1:B:294:LYS:HG2	19	1.78
(1,679)	1:B:290:LEU:HD13	1:B:294:LYS:HG2	19	1.78
(1,658)	1:B:293:LEU:HD11	1:B:294:LYS:HG3	10	1.78
(1,658)	1:B:293:LEU:HD12	1:B:294:LYS:HG3	10	1.78
(1,658)	1:B:293:LEU:HD13	1:B:294:LYS:HG3	10	1.78
(1,630)	1:B:252:VAL:HG21	1:B:279:ILE:HA	9	1.78
(1,630)	1:B:252:VAL:HG22	1:B:279:ILE:HA	9	1.78
(1,630)	1:B:252:VAL:HG23	1:B:279:ILE:HA	9	1.78
(1,34)	1:B:312:ASN:HA	1:B:315:LEU:HD21	4	1.78
(1,34)	1:B:312:ASN:HA	1:B:315:LEU:HD22	4	1.78
(1,34)	1:B:312:ASN:HA	1:B:315:LEU:HD23	4	1.78
(1,101)	1:A:93:LEU:HD11	1:A:97:TRP:HA	11	1.78
(1,101)	1:A:93:LEU:HD12	1:A:97:TRP:HA	11	1.78
(1,101)	1:A:93:LEU:HD13	1:A:97:TRP:HA	11	1.78
(1,627)	1:A:52:VAL:HG21	1:A:54:VAL:HA	15	1.77
(1,627)	1:A:52:VAL:HG22	1:A:54:VAL:HA	15	1.77

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,627)	1:A:52:VAL:HG23	1:A:54:VAL:HA	15	1.77
(1,610)	1:B:249:GLY:HA3	1:B:250:GLN:HB2	2	1.77
(1,588)	1:B:222:THR:H	1:B:223:ARG:HD3	14	1.77
(1,1216)	1:B:231:SER:H	1:B:252:VAL:HG11	4	1.77
(1,1216)	1:B:231:SER:H	1:B:252:VAL:HG12	4	1.77
(1,1216)	1:B:231:SER:H	1:B:252:VAL:HG13	4	1.77
(1,629)	1:B:252:VAL:HG21	1:B:254:VAL:HA	4	1.76
(1,629)	1:B:252:VAL:HG22	1:B:254:VAL:HA	4	1.76
(1,629)	1:B:252:VAL:HG23	1:B:254:VAL:HA	4	1.76
(1,627)	1:A:52:VAL:HG21	1:A:54:VAL:HA	13	1.76
(1,627)	1:A:52:VAL:HG22	1:A:54:VAL:HA	13	1.76
(1,627)	1:A:52:VAL:HG23	1:A:54:VAL:HA	13	1.76
(1,647)	1:A:102:ARG:HG2	1:A:125:VAL:HA	8	1.75
(1,677)	1:A:90:LEU:HD11	1:A:94:LYS:HG2	15	1.74
(1,677)	1:A:90:LEU:HD12	1:A:94:LYS:HG2	15	1.74
(1,677)	1:A:90:LEU:HD13	1:A:94:LYS:HG2	15	1.74
(1,628)	1:A:52:VAL:HG21	1:A:79:ILE:HA	11	1.74
(1,628)	1:A:52:VAL:HG22	1:A:79:ILE:HA	11	1.74
(1,628)	1:A:52:VAL:HG23	1:A:79:ILE:HA	11	1.74
(1,610)	1:B:249:GLY:HA3	1:B:250:GLN:HB2	20	1.74
(1,679)	1:B:290:LEU:HD11	1:B:294:LYS:HG2	10	1.73
(1,679)	1:B:290:LEU:HD12	1:B:294:LYS:HG2	10	1.73
(1,679)	1:B:290:LEU:HD13	1:B:294:LYS:HG2	10	1.73
(1,628)	1:A:52:VAL:HG21	1:A:79:ILE:HA	14	1.73
(1,628)	1:A:52:VAL:HG22	1:A:79:ILE:HA	14	1.73
(1,628)	1:A:52:VAL:HG23	1:A:79:ILE:HA	14	1.73
(1,627)	1:A:52:VAL:HG21	1:A:54:VAL:HA	1	1.72
(1,627)	1:A:52:VAL:HG22	1:A:54:VAL:HA	1	1.72
(1,627)	1:A:52:VAL:HG23	1:A:54:VAL:HA	1	1.72
(1,627)	1:A:52:VAL:HG21	1:A:54:VAL:HA	4	1.72
(1,627)	1:A:52:VAL:HG22	1:A:54:VAL:HA	4	1.72
(1,627)	1:A:52:VAL:HG23	1:A:54:VAL:HA	4	1.72
(1,497)	1:A:20:ASP:HB2	1:A:23:ARG:HD3	18	1.71
(1,905)	1:B:303:ASN:H	1:B:324:ILE:HG12	4	1.7
(1,460)	1:B:302:ARG:HG3	1:B:305:ASP:HB2	1	1.7
(1,498)	1:B:220:ASP:HB2	1:B:223:ARG:HD3	18	1.69
(1,1249)	1:A:70:VAL:HG11	1:A:72:MET:H	12	1.69
(1,1249)	1:A:70:VAL:HG12	1:A:72:MET:H	12	1.69
(1,1249)	1:A:70:VAL:HG13	1:A:72:MET:H	12	1.69
(1,1216)	1:B:231:SER:H	1:B:252:VAL:HG11	3	1.68
(1,1216)	1:B:231:SER:H	1:B:252:VAL:HG12	3	1.68
(1,1216)	1:B:231:SER:H	1:B:252:VAL:HG13	3	1.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,97)	1:B:232:LEU:HD11	1:B:234:ARG:HA	11	1.66
(1,97)	1:B:232:LEU:HD12	1:B:234:ARG:HA	11	1.66
(1,97)	1:B:232:LEU:HD13	1:B:234:ARG:HA	11	1.66
(1,95)	1:A:32:LEU:HD11	1:A:34:ARG:HA	3	1.66
(1,95)	1:A:32:LEU:HD12	1:A:34:ARG:HA	3	1.66
(1,95)	1:A:32:LEU:HD13	1:A:34:ARG:HA	3	1.66
(1,902)	1:A:103:ASN:H	1:A:124:ILE:HG12	13	1.66
(1,548)	1:A:69:CYS:HB3	1:A:70:VAL:HB	20	1.66
(1,97)	1:B:232:LEU:HD11	1:B:234:ARG:HA	3	1.65
(1,97)	1:B:232:LEU:HD12	1:B:234:ARG:HA	3	1.65
(1,97)	1:B:232:LEU:HD13	1:B:234:ARG:HA	3	1.65
(1,799)	1:A:112:ASN:H	1:A:115:LEU:HD21	14	1.65
(1,799)	1:A:112:ASN:H	1:A:115:LEU:HD22	14	1.65
(1,799)	1:A:112:ASN:H	1:A:115:LEU:HD23	14	1.65
(1,457)	1:A:102:ARG:HG3	1:A:105:ASP:HB2	1	1.65
(1,648)	1:B:302:ARG:HG2	1:B:325:VAL:HA	1	1.64
(1,102)	1:B:293:LEU:HD11	1:B:297:TRP:HA	15	1.64
(1,102)	1:B:293:LEU:HD12	1:B:297:TRP:HA	15	1.64
(1,102)	1:B:293:LEU:HD13	1:B:297:TRP:HA	15	1.64
(1,679)	1:B:290:LEU:HD11	1:B:294:LYS:HG2	4	1.63
(1,679)	1:B:290:LEU:HD12	1:B:294:LYS:HG2	4	1.63
(1,679)	1:B:290:LEU:HD13	1:B:294:LYS:HG2	4	1.63
(1,102)	1:B:293:LEU:HD11	1:B:297:TRP:HA	10	1.63
(1,102)	1:B:293:LEU:HD12	1:B:297:TRP:HA	10	1.63
(1,102)	1:B:293:LEU:HD13	1:B:297:TRP:HA	10	1.63
(1,800)	1:B:312:ASN:H	1:B:315:LEU:HD21	14	1.62
(1,800)	1:B:312:ASN:H	1:B:315:LEU:HD22	14	1.62
(1,800)	1:B:312:ASN:H	1:B:315:LEU:HD23	14	1.62
(1,677)	1:A:90:LEU:HD11	1:A:94:LYS:HG2	10	1.62
(1,677)	1:A:90:LEU:HD12	1:A:94:LYS:HG2	10	1.62
(1,677)	1:A:90:LEU:HD13	1:A:94:LYS:HG2	10	1.62
(1,1214)	1:A:31:SER:H	1:A:52:VAL:HG11	13	1.62
(1,1214)	1:A:31:SER:H	1:A:52:VAL:HG12	13	1.62
(1,1214)	1:A:31:SER:H	1:A:52:VAL:HG13	13	1.62
(1,677)	1:A:90:LEU:HD11	1:A:94:LYS:HG2	4	1.61
(1,677)	1:A:90:LEU:HD12	1:A:94:LYS:HG2	4	1.61
(1,677)	1:A:90:LEU:HD13	1:A:94:LYS:HG2	4	1.61
(1,629)	1:B:252:VAL:HG21	1:B:254:VAL:HA	18	1.61
(1,629)	1:B:252:VAL:HG22	1:B:254:VAL:HA	18	1.61
(1,629)	1:B:252:VAL:HG23	1:B:254:VAL:HA	18	1.61
(1,905)	1:B:303:ASN:H	1:B:324:ILE:HG12	5	1.6
(1,1214)	1:A:31:SER:H	1:A:52:VAL:HG11	1	1.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1214)	1:A:31:SER:H	1:A:52:VAL:HG12	1	1.59
(1,1214)	1:A:31:SER:H	1:A:52:VAL:HG13	1	1.59
(1,647)	1:A:102:ARG:HG2	1:A:125:VAL:HA	1	1.58
(1,497)	1:A:20:ASP:HB2	1:A:23:ARG:HD3	14	1.58
(1,1216)	1:B:231:SER:H	1:B:252:VAL:HG11	1	1.58
(1,1216)	1:B:231:SER:H	1:B:252:VAL:HG12	1	1.58
(1,1216)	1:B:231:SER:H	1:B:252:VAL:HG13	1	1.58
(1,799)	1:A:112:ASN:H	1:A:115:LEU:HD21	15	1.57
(1,799)	1:A:112:ASN:H	1:A:115:LEU:HD22	15	1.57
(1,799)	1:A:112:ASN:H	1:A:115:LEU:HD23	15	1.57
(1,905)	1:B:303:ASN:H	1:B:324:ILE:HG12	17	1.56
(1,498)	1:B:220:ASP:HB2	1:B:223:ARG:HD3	7	1.56
(1,1214)	1:A:31:SER:H	1:A:52:VAL:HG11	14	1.56
(1,1214)	1:A:31:SER:H	1:A:52:VAL:HG12	14	1.56
(1,1214)	1:A:31:SER:H	1:A:52:VAL:HG13	14	1.56
(1,904)	1:B:303:ASN:H	1:B:325:VAL:HG21	17	1.55
(1,904)	1:B:303:ASN:H	1:B:325:VAL:HG22	17	1.55
(1,904)	1:B:303:ASN:H	1:B:325:VAL:HG23	17	1.55
(1,800)	1:B:312:ASN:H	1:B:315:LEU:HD21	15	1.55
(1,800)	1:B:312:ASN:H	1:B:315:LEU:HD22	15	1.55
(1,800)	1:B:312:ASN:H	1:B:315:LEU:HD23	15	1.55
(1,630)	1:B:252:VAL:HG21	1:B:279:ILE:HA	13	1.55
(1,630)	1:B:252:VAL:HG22	1:B:279:ILE:HA	13	1.55
(1,630)	1:B:252:VAL:HG23	1:B:279:ILE:HA	13	1.55
(1,629)	1:B:252:VAL:HG21	1:B:254:VAL:HA	16	1.54
(1,629)	1:B:252:VAL:HG22	1:B:254:VAL:HA	16	1.54
(1,629)	1:B:252:VAL:HG23	1:B:254:VAL:HA	16	1.54
(1,462)	1:B:303:ASN:HA	1:B:305:ASP:HB2	1	1.53
(1,461)	1:A:103:ASN:HA	1:A:105:ASP:HB2	1	1.53
(1,1214)	1:A:31:SER:H	1:A:52:VAL:HG11	20	1.53
(1,1214)	1:A:31:SER:H	1:A:52:VAL:HG12	20	1.53
(1,1214)	1:A:31:SER:H	1:A:52:VAL:HG13	20	1.53
(1,1108)	1:A:75:GLU:H	1:B:244:LEU:HD11	20	1.53
(1,1108)	1:A:75:GLU:H	1:B:244:LEU:HD12	20	1.53
(1,1108)	1:A:75:GLU:H	1:B:244:LEU:HD13	20	1.53
(1,902)	1:A:103:ASN:H	1:A:124:ILE:HG12	17	1.52
(1,628)	1:A:52:VAL:HG21	1:A:79:ILE:HA	17	1.52
(1,628)	1:A:52:VAL:HG22	1:A:79:ILE:HA	17	1.52
(1,628)	1:A:52:VAL:HG23	1:A:79:ILE:HA	17	1.52
(1,1311)	1:A:32:LEU:HD11	1:A:34:ARG:H	20	1.52
(1,1311)	1:A:32:LEU:HD12	1:A:34:ARG:H	20	1.52
(1,1311)	1:A:32:LEU:HD13	1:A:34:ARG:H	20	1.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,630)	1:B:252:VAL:HG21	1:B:279:ILE:HA	11	1.5
(1,630)	1:B:252:VAL:HG22	1:B:279:ILE:HA	11	1.5
(1,630)	1:B:252:VAL:HG23	1:B:279:ILE:HA	11	1.5
(1,550)	1:B:269:CYS:HB3	1:B:270:VAL:HB	17	1.5
(1,102)	1:B:293:LEU:HD11	1:B:297:TRP:HA	6	1.49
(1,102)	1:B:293:LEU:HD12	1:B:297:TRP:HA	6	1.49
(1,102)	1:B:293:LEU:HD13	1:B:297:TRP:HA	6	1.49
(1,514)	1:A:125:VAL:HB	1:B:205:PRO:HB2	8	1.48
(1,30)	1:B:232:LEU:HD11	1:B:233:LEU:HA	8	1.48
(1,30)	1:B:232:LEU:HD12	1:B:233:LEU:HA	8	1.48
(1,30)	1:B:232:LEU:HD13	1:B:233:LEU:HA	8	1.48
(1,547)	1:A:20:ASP:HB2	1:A:21:PRO:HB2	20	1.47
(1,1107)	1:A:44:LEU:HD11	1:B:275:GLU:H	20	1.47
(1,1107)	1:A:44:LEU:HD12	1:B:275:GLU:H	20	1.47
(1,1107)	1:A:44:LEU:HD13	1:B:275:GLU:H	20	1.47
(1,630)	1:B:252:VAL:HG21	1:B:279:ILE:HA	17	1.46
(1,630)	1:B:252:VAL:HG22	1:B:279:ILE:HA	17	1.46
(1,630)	1:B:252:VAL:HG23	1:B:279:ILE:HA	17	1.46
(1,549)	1:B:220:ASP:HB2	1:B:221:PRO:HB2	8	1.46
(1,549)	1:B:220:ASP:HB2	1:B:221:PRO:HB2	20	1.46
(1,514)	1:A:125:VAL:HB	1:B:205:PRO:HB2	7	1.46
(1,224)	1:B:315:LEU:HD21	1:B:316:GLY:HA2	13	1.46
(1,224)	1:B:315:LEU:HD22	1:B:316:GLY:HA2	13	1.46
(1,224)	1:B:315:LEU:HD23	1:B:316:GLY:HA2	13	1.46
(1,102)	1:B:293:LEU:HD11	1:B:297:TRP:HA	5	1.46
(1,102)	1:B:293:LEU:HD12	1:B:297:TRP:HA	5	1.46
(1,102)	1:B:293:LEU:HD13	1:B:297:TRP:HA	5	1.46
(1,799)	1:A:112:ASN:H	1:A:115:LEU:HD21	4	1.45
(1,799)	1:A:112:ASN:H	1:A:115:LEU:HD22	4	1.45
(1,799)	1:A:112:ASN:H	1:A:115:LEU:HD23	4	1.45
(1,630)	1:B:252:VAL:HG21	1:B:279:ILE:HA	3	1.45
(1,630)	1:B:252:VAL:HG22	1:B:279:ILE:HA	3	1.45
(1,630)	1:B:252:VAL:HG23	1:B:279:ILE:HA	3	1.45
(1,627)	1:A:52:VAL:HG21	1:A:54:VAL:HA	7	1.45
(1,627)	1:A:52:VAL:HG22	1:A:54:VAL:HA	7	1.45
(1,627)	1:A:52:VAL:HG23	1:A:54:VAL:HA	7	1.45
(1,549)	1:B:220:ASP:HB2	1:B:221:PRO:HB2	6	1.45
(1,547)	1:A:20:ASP:HB2	1:A:21:PRO:HB2	13	1.45
(1,513)	1:A:5:PRO:HB2	1:B:325:VAL:HB	8	1.45
(1,29)	1:A:32:LEU:HD11	1:A:33:LEU:HA	7	1.45
(1,29)	1:A:32:LEU:HD12	1:A:33:LEU:HA	7	1.45
(1,29)	1:A:32:LEU:HD13	1:A:33:LEU:HA	7	1.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,800)	1:B:312:ASN:H	1:B:315:LEU:HD21	4	1.44
(1,800)	1:B:312:ASN:H	1:B:315:LEU:HD22	4	1.44
(1,800)	1:B:312:ASN:H	1:B:315:LEU:HD23	4	1.44
(1,629)	1:B:252:VAL:HG21	1:B:254:VAL:HA	3	1.44
(1,629)	1:B:252:VAL:HG22	1:B:254:VAL:HA	3	1.44
(1,629)	1:B:252:VAL:HG23	1:B:254:VAL:HA	3	1.44
(1,547)	1:A:20:ASP:HB2	1:A:21:PRO:HB2	6	1.44
(1,29)	1:A:32:LEU:HD11	1:A:33:LEU:HA	8	1.44
(1,29)	1:A:32:LEU:HD12	1:A:33:LEU:HA	8	1.44
(1,29)	1:A:32:LEU:HD13	1:A:33:LEU:HA	8	1.44
(1,101)	1:A:93:LEU:HD11	1:A:97:TRP:HA	5	1.44
(1,101)	1:A:93:LEU:HD12	1:A:97:TRP:HA	5	1.44
(1,101)	1:A:93:LEU:HD13	1:A:97:TRP:HA	5	1.44
(1,224)	1:B:315:LEU:HD21	1:B:316:GLY:HA2	4	1.43
(1,224)	1:B:315:LEU:HD22	1:B:316:GLY:HA2	4	1.43
(1,224)	1:B:315:LEU:HD23	1:B:316:GLY:HA2	4	1.43
(1,223)	1:A:115:LEU:HD21	1:A:116:GLY:HA2	4	1.43
(1,223)	1:A:115:LEU:HD22	1:A:116:GLY:HA2	4	1.43
(1,223)	1:A:115:LEU:HD23	1:A:116:GLY:HA2	4	1.43
(1,905)	1:B:303:ASN:H	1:B:324:ILE:HG12	15	1.42
(1,549)	1:B:220:ASP:HB2	1:B:221:PRO:HB2	13	1.42
(1,547)	1:A:20:ASP:HB2	1:A:21:PRO:HB2	5	1.42
(1,547)	1:A:20:ASP:HB2	1:A:21:PRO:HB2	18	1.42
(1,461)	1:A:103:ASN:HA	1:A:105:ASP:HB2	7	1.42
(1,30)	1:B:232:LEU:HD11	1:B:233:LEU:HA	7	1.42
(1,30)	1:B:232:LEU:HD12	1:B:233:LEU:HA	7	1.42
(1,30)	1:B:232:LEU:HD13	1:B:233:LEU:HA	7	1.42
(1,224)	1:B:315:LEU:HD21	1:B:316:GLY:HA2	2	1.42
(1,224)	1:B:315:LEU:HD22	1:B:316:GLY:HA2	2	1.42
(1,224)	1:B:315:LEU:HD23	1:B:316:GLY:HA2	2	1.42
(1,223)	1:A:115:LEU:HD21	1:A:116:GLY:HA2	2	1.42
(1,223)	1:A:115:LEU:HD22	1:A:116:GLY:HA2	2	1.42
(1,223)	1:A:115:LEU:HD23	1:A:116:GLY:HA2	2	1.42
(1,223)	1:A:115:LEU:HD21	1:A:116:GLY:HA2	15	1.42
(1,223)	1:A:115:LEU:HD22	1:A:116:GLY:HA2	15	1.42
(1,223)	1:A:115:LEU:HD23	1:A:116:GLY:HA2	15	1.42
(1,101)	1:A:93:LEU:HD11	1:A:97:TRP:HA	16	1.42
(1,101)	1:A:93:LEU:HD12	1:A:97:TRP:HA	16	1.42
(1,101)	1:A:93:LEU:HD13	1:A:97:TRP:HA	16	1.42
(1,905)	1:B:303:ASN:H	1:B:324:ILE:HG12	8	1.41
(1,647)	1:A:102:ARG:HG2	1:A:125:VAL:HA	6	1.41
(1,630)	1:B:252:VAL:HG21	1:B:279:ILE:HA	10	1.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,630)	1:B:252:VAL:HG22	1:B:279:ILE:HA	10	1.41
(1,630)	1:B:252:VAL:HG23	1:B:279:ILE:HA	10	1.41
(1,549)	1:B:220:ASP:HB2	1:B:221:PRO:HB2	5	1.41
(1,549)	1:B:220:ASP:HB2	1:B:221:PRO:HB2	18	1.41
(1,224)	1:B:315:LEU:HD21	1:B:316:GLY:HA2	14	1.41
(1,224)	1:B:315:LEU:HD22	1:B:316:GLY:HA2	14	1.41
(1,224)	1:B:315:LEU:HD23	1:B:316:GLY:HA2	14	1.41
(1,224)	1:B:315:LEU:HD21	1:B:316:GLY:HA2	15	1.41
(1,224)	1:B:315:LEU:HD22	1:B:316:GLY:HA2	15	1.41
(1,224)	1:B:315:LEU:HD23	1:B:316:GLY:HA2	15	1.41
(1,223)	1:A:115:LEU:HD21	1:A:116:GLY:HA2	14	1.41
(1,223)	1:A:115:LEU:HD22	1:A:116:GLY:HA2	14	1.41
(1,223)	1:A:115:LEU:HD23	1:A:116:GLY:HA2	14	1.41
(1,677)	1:A:90:LEU:HD11	1:A:94:LYS:HG2	1	1.4
(1,677)	1:A:90:LEU:HD12	1:A:94:LYS:HG2	1	1.4
(1,677)	1:A:90:LEU:HD13	1:A:94:LYS:HG2	1	1.4
(1,549)	1:B:220:ASP:HB2	1:B:221:PRO:HB2	3	1.4
(1,547)	1:A:20:ASP:HB2	1:A:21:PRO:HB2	3	1.4
(1,547)	1:A:20:ASP:HB2	1:A:21:PRO:HB2	9	1.4
(1,513)	1:A:5:PRO:HB2	1:B:325:VAL:HB	7	1.4
(1,462)	1:B:303:ASN:HA	1:B:305:ASP:HB2	7	1.4
(1,224)	1:B:315:LEU:HD21	1:B:316:GLY:HA2	18	1.4
(1,224)	1:B:315:LEU:HD22	1:B:316:GLY:HA2	18	1.4
(1,224)	1:B:315:LEU:HD23	1:B:316:GLY:HA2	18	1.4
(1,223)	1:A:115:LEU:HD21	1:A:116:GLY:HA2	18	1.4
(1,223)	1:A:115:LEU:HD22	1:A:116:GLY:HA2	18	1.4
(1,223)	1:A:115:LEU:HD23	1:A:116:GLY:HA2	18	1.4
(1,905)	1:B:303:ASN:H	1:B:324:ILE:HG12	12	1.39
(1,549)	1:B:220:ASP:HB2	1:B:221:PRO:HB2	9	1.39
(1,498)	1:B:220:ASP:HB2	1:B:223:ARG:HD3	10	1.39
(1,1214)	1:A:31:SER:H	1:A:52:VAL:HG11	9	1.39
(1,1214)	1:A:31:SER:H	1:A:52:VAL:HG12	9	1.39
(1,1214)	1:A:31:SER:H	1:A:52:VAL:HG13	9	1.39
(1,97)	1:B:232:LEU:HD11	1:B:234:ARG:HA	7	1.38
(1,97)	1:B:232:LEU:HD12	1:B:234:ARG:HA	7	1.38
(1,97)	1:B:232:LEU:HD13	1:B:234:ARG:HA	7	1.38
(1,630)	1:B:252:VAL:HG21	1:B:279:ILE:HA	16	1.38
(1,630)	1:B:252:VAL:HG22	1:B:279:ILE:HA	16	1.38
(1,630)	1:B:252:VAL:HG23	1:B:279:ILE:HA	16	1.38
(1,497)	1:A:20:ASP:HB2	1:A:23:ARG:HD3	7	1.38
(1,224)	1:B:315:LEU:HD21	1:B:316:GLY:HA2	12	1.38
(1,224)	1:B:315:LEU:HD22	1:B:316:GLY:HA2	12	1.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,224)	1:B:315:LEU:HD23	1:B:316:GLY:HA2	12	1.38
(1,101)	1:A:93:LEU:HD11	1:A:97:TRP:HA	15	1.38
(1,101)	1:A:93:LEU:HD12	1:A:97:TRP:HA	15	1.38
(1,101)	1:A:93:LEU:HD13	1:A:97:TRP:HA	15	1.38
(1,630)	1:B:252:VAL:HG21	1:B:279:ILE:HA	1	1.37
(1,630)	1:B:252:VAL:HG22	1:B:279:ILE:HA	1	1.37
(1,630)	1:B:252:VAL:HG23	1:B:279:ILE:HA	1	1.37
(1,514)	1:A:125:VAL:HB	1:B:205:PRO:HB2	2	1.37
(1,905)	1:B:303:ASN:H	1:B:324:ILE:HG12	2	1.36
(1,902)	1:A:103:ASN:H	1:A:124:ILE:HG12	2	1.36
(1,547)	1:A:20:ASP:HB2	1:A:21:PRO:HB2	8	1.36
(1,497)	1:A:20:ASP:HB2	1:A:23:ARG:HD3	5	1.36
(1,549)	1:B:220:ASP:HB2	1:B:221:PRO:HB2	2	1.35
(1,223)	1:A:115:LEU:HD21	1:A:116:GLY:HA2	12	1.35
(1,223)	1:A:115:LEU:HD22	1:A:116:GLY:HA2	12	1.35
(1,223)	1:A:115:LEU:HD23	1:A:116:GLY:HA2	12	1.35
(1,549)	1:B:220:ASP:HB2	1:B:221:PRO:HB2	7	1.34
(1,547)	1:A:20:ASP:HB2	1:A:21:PRO:HB2	2	1.34
(1,457)	1:A:102:ARG:HG3	1:A:105:ASP:HB2	6	1.34
(1,393)	1:A:124:ILE:HD11	1:A:125:VAL:HG21	1	1.34
(1,393)	1:A:124:ILE:HD11	1:A:125:VAL:HG22	1	1.34
(1,393)	1:A:124:ILE:HD11	1:A:125:VAL:HG23	1	1.34
(1,393)	1:A:124:ILE:HD12	1:A:125:VAL:HG21	1	1.34
(1,393)	1:A:124:ILE:HD12	1:A:125:VAL:HG22	1	1.34
(1,393)	1:A:124:ILE:HD12	1:A:125:VAL:HG23	1	1.34
(1,393)	1:A:124:ILE:HD13	1:A:125:VAL:HG21	1	1.34
(1,393)	1:A:124:ILE:HD13	1:A:125:VAL:HG22	1	1.34
(1,393)	1:A:124:ILE:HD13	1:A:125:VAL:HG23	1	1.34
(1,1108)	1:A:75:GLU:H	1:B:244:LEU:HD11	16	1.34
(1,1108)	1:A:75:GLU:H	1:B:244:LEU:HD12	16	1.34
(1,1108)	1:A:75:GLU:H	1:B:244:LEU:HD13	16	1.34
(1,902)	1:A:103:ASN:H	1:A:124:ILE:HG12	7	1.33
(1,902)	1:A:103:ASN:H	1:A:124:ILE:HG12	12	1.33
(1,498)	1:B:220:ASP:HB2	1:B:223:ARG:HD3	5	1.33
(1,160)	1:B:287:ALA:HA	1:B:290:LEU:HD21	3	1.33
(1,160)	1:B:287:ALA:HA	1:B:290:LEU:HD22	3	1.33
(1,160)	1:B:287:ALA:HA	1:B:290:LEU:HD23	3	1.33
(1,159)	1:A:87:ALA:HA	1:A:90:LEU:HD21	1	1.33
(1,159)	1:A:87:ALA:HA	1:A:90:LEU:HD22	1	1.33
(1,159)	1:A:87:ALA:HA	1:A:90:LEU:HD23	1	1.33
(1,159)	1:A:87:ALA:HA	1:A:90:LEU:HD21	3	1.33
(1,159)	1:A:87:ALA:HA	1:A:90:LEU:HD22	3	1.33

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,159)	1:A:87:ALA:HA	1:A:90:LEU:HD23	3	1.33
(1,1214)	1:A:31:SER:H	1:A:52:VAL:HG11	18	1.33
(1,1214)	1:A:31:SER:H	1:A:52:VAL:HG12	18	1.33
(1,1214)	1:A:31:SER:H	1:A:52:VAL:HG13	18	1.33
(1,930)	1:A:50:GLN:H	1:A:82:VAL:HG11	9	1.32
(1,930)	1:A:50:GLN:H	1:A:82:VAL:HG12	9	1.32
(1,930)	1:A:50:GLN:H	1:A:82:VAL:HG13	9	1.32
(1,905)	1:B:303:ASN:H	1:B:324:ILE:HG12	7	1.32
(1,549)	1:B:220:ASP:HB2	1:B:221:PRO:HB2	11	1.32
(1,513)	1:A:5:PRO:HB2	1:B:325:VAL:HB	2	1.32
(1,1108)	1:A:75:GLU:H	1:B:244:LEU:HD11	13	1.32
(1,1108)	1:A:75:GLU:H	1:B:244:LEU:HD12	13	1.32
(1,1108)	1:A:75:GLU:H	1:B:244:LEU:HD13	13	1.32
(1,1107)	1:A:44:LEU:HD11	1:B:275:GLU:H	16	1.32
(1,1107)	1:A:44:LEU:HD12	1:B:275:GLU:H	16	1.32
(1,1107)	1:A:44:LEU:HD13	1:B:275:GLU:H	16	1.32
(1,102)	1:B:293:LEU:HD11	1:B:297:TRP:HA	9	1.32
(1,102)	1:B:293:LEU:HD12	1:B:297:TRP:HA	9	1.32
(1,102)	1:B:293:LEU:HD13	1:B:297:TRP:HA	9	1.32
(1,97)	1:B:232:LEU:HD11	1:B:234:ARG:HA	8	1.31
(1,97)	1:B:232:LEU:HD12	1:B:234:ARG:HA	8	1.31
(1,97)	1:B:232:LEU:HD13	1:B:234:ARG:HA	8	1.31
(1,677)	1:A:90:LEU:HD11	1:A:94:LYS:HG2	16	1.31
(1,677)	1:A:90:LEU:HD12	1:A:94:LYS:HG2	16	1.31
(1,677)	1:A:90:LEU:HD13	1:A:94:LYS:HG2	16	1.31
(1,547)	1:A:20:ASP:HB2	1:A:21:PRO:HB2	11	1.31
(1,1268)	1:B:217:VAL:HG11	1:B:219:SER:H	8	1.31
(1,1268)	1:B:217:VAL:HG12	1:B:219:SER:H	8	1.31
(1,1268)	1:B:217:VAL:HG13	1:B:219:SER:H	8	1.31
(1,577)	1:A:93:LEU:HD11	1:A:94:LYS:HB2	16	1.3
(1,577)	1:A:93:LEU:HD11	1:A:94:LYS:HB3	16	1.3
(1,577)	1:A:93:LEU:HD12	1:A:94:LYS:HB2	16	1.3
(1,577)	1:A:93:LEU:HD12	1:A:94:LYS:HB3	16	1.3
(1,577)	1:A:93:LEU:HD13	1:A:94:LYS:HB2	16	1.3
(1,577)	1:A:93:LEU:HD13	1:A:94:LYS:HB3	16	1.3
(1,497)	1:A:20:ASP:HB2	1:A:23:ARG:HD3	10	1.3
(1,34)	1:B:312:ASN:HA	1:B:315:LEU:HD21	11	1.29
(1,34)	1:B:312:ASN:HA	1:B:315:LEU:HD22	11	1.29
(1,34)	1:B:312:ASN:HA	1:B:315:LEU:HD23	11	1.29
(1,1216)	1:B:231:SER:H	1:B:252:VAL:HG11	10	1.29
(1,1216)	1:B:231:SER:H	1:B:252:VAL:HG12	10	1.29
(1,1216)	1:B:231:SER:H	1:B:252:VAL:HG13	10	1.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1107)	1:A:44:LEU:HD11	1:B:275:GLU:H	10	1.29
(1,1107)	1:A:44:LEU:HD12	1:B:275:GLU:H	10	1.29
(1,1107)	1:A:44:LEU:HD13	1:B:275:GLU:H	10	1.29
(1,95)	1:A:32:LEU:HD11	1:A:34:ARG:HA	8	1.28
(1,95)	1:A:32:LEU:HD12	1:A:34:ARG:HA	8	1.28
(1,95)	1:A:32:LEU:HD13	1:A:34:ARG:HA	8	1.28
(1,95)	1:A:32:LEU:HD11	1:A:34:ARG:HA	19	1.28
(1,95)	1:A:32:LEU:HD12	1:A:34:ARG:HA	19	1.28
(1,95)	1:A:32:LEU:HD13	1:A:34:ARG:HA	19	1.28
(1,930)	1:A:50:GLN:H	1:A:82:VAL:HG11	7	1.28
(1,930)	1:A:50:GLN:H	1:A:82:VAL:HG12	7	1.28
(1,930)	1:A:50:GLN:H	1:A:82:VAL:HG13	7	1.28
(1,667)	1:A:88:GLU:HB2	1:A:89:ASN:HB2	1	1.28
(1,667)	1:A:88:GLU:HB2	1:A:89:ASN:HB3	1	1.28
(1,95)	1:A:32:LEU:HD11	1:A:34:ARG:HA	1	1.27
(1,95)	1:A:32:LEU:HD12	1:A:34:ARG:HA	1	1.27
(1,95)	1:A:32:LEU:HD13	1:A:34:ARG:HA	1	1.27
(1,628)	1:A:52:VAL:HG21	1:A:79:ILE:HA	6	1.27
(1,628)	1:A:52:VAL:HG22	1:A:79:ILE:HA	6	1.27
(1,628)	1:A:52:VAL:HG23	1:A:79:ILE:HA	6	1.27
(1,497)	1:A:20:ASP:HB2	1:A:23:ARG:HD3	4	1.27
(1,1216)	1:B:231:SER:H	1:B:252:VAL:HG11	20	1.27
(1,1216)	1:B:231:SER:H	1:B:252:VAL:HG12	20	1.27
(1,1216)	1:B:231:SER:H	1:B:252:VAL:HG13	20	1.27
(1,1108)	1:A:75:GLU:H	1:B:244:LEU:HD11	10	1.27
(1,1108)	1:A:75:GLU:H	1:B:244:LEU:HD12	10	1.27
(1,1108)	1:A:75:GLU:H	1:B:244:LEU:HD13	10	1.27
(1,95)	1:A:32:LEU:HD11	1:A:34:ARG:HA	14	1.26
(1,95)	1:A:32:LEU:HD12	1:A:34:ARG:HA	14	1.26
(1,95)	1:A:32:LEU:HD13	1:A:34:ARG:HA	14	1.26
(1,628)	1:A:52:VAL:HG21	1:A:79:ILE:HA	13	1.26
(1,628)	1:A:52:VAL:HG22	1:A:79:ILE:HA	13	1.26
(1,628)	1:A:52:VAL:HG23	1:A:79:ILE:HA	13	1.26
(1,547)	1:A:20:ASP:HB2	1:A:21:PRO:HB2	15	1.26
(1,498)	1:B:220:ASP:HB2	1:B:223:ARG:HD3	4	1.26
(1,95)	1:A:32:LEU:HD11	1:A:34:ARG:HA	18	1.25
(1,95)	1:A:32:LEU:HD12	1:A:34:ARG:HA	18	1.25
(1,95)	1:A:32:LEU:HD13	1:A:34:ARG:HA	18	1.25
(1,629)	1:B:252:VAL:HG21	1:B:254:VAL:HA	8	1.25
(1,629)	1:B:252:VAL:HG22	1:B:254:VAL:HA	8	1.25
(1,629)	1:B:252:VAL:HG23	1:B:254:VAL:HA	8	1.25
(1,578)	1:B:293:LEU:HD11	1:B:294:LYS:HB2	12	1.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,578)	1:B:293:LEU:HD11	1:B:294:LYS:HB3	12	1.25
(1,578)	1:B:293:LEU:HD12	1:B:294:LYS:HB2	12	1.25
(1,578)	1:B:293:LEU:HD12	1:B:294:LYS:HB3	12	1.25
(1,578)	1:B:293:LEU:HD13	1:B:294:LYS:HB2	12	1.25
(1,578)	1:B:293:LEU:HD13	1:B:294:LYS:HB3	12	1.25
(1,260)	1:B:228:PHE:HA	1:B:252:VAL:HB	15	1.25
(1,932)	1:B:250:GLN:H	1:B:282:VAL:HG11	12	1.24
(1,932)	1:B:250:GLN:H	1:B:282:VAL:HG12	12	1.24
(1,932)	1:B:250:GLN:H	1:B:282:VAL:HG13	12	1.24
(1,577)	1:A:93:LEU:HD11	1:A:94:LYS:HB2	12	1.24
(1,577)	1:A:93:LEU:HD11	1:A:94:LYS:HB3	12	1.24
(1,577)	1:A:93:LEU:HD12	1:A:94:LYS:HB2	12	1.24
(1,577)	1:A:93:LEU:HD12	1:A:94:LYS:HB3	12	1.24
(1,577)	1:A:93:LEU:HD13	1:A:94:LYS:HB2	12	1.24
(1,577)	1:A:93:LEU:HD13	1:A:94:LYS:HB3	12	1.24
(1,1281)	1:A:93:LEU:HD11	1:A:96:GLU:H	6	1.24
(1,1281)	1:A:93:LEU:HD12	1:A:96:GLU:H	6	1.24
(1,1281)	1:A:93:LEU:HD13	1:A:96:GLU:H	6	1.24
(1,1107)	1:A:44:LEU:HD11	1:B:275:GLU:H	13	1.24
(1,1107)	1:A:44:LEU:HD12	1:B:275:GLU:H	13	1.24
(1,1107)	1:A:44:LEU:HD13	1:B:275:GLU:H	13	1.24
(1,101)	1:A:93:LEU:HD11	1:A:97:TRP:HA	9	1.24
(1,101)	1:A:93:LEU:HD12	1:A:97:TRP:HA	9	1.24
(1,101)	1:A:93:LEU:HD13	1:A:97:TRP:HA	9	1.24
(1,95)	1:A:32:LEU:HD11	1:A:34:ARG:HA	9	1.23
(1,95)	1:A:32:LEU:HD12	1:A:34:ARG:HA	9	1.23
(1,95)	1:A:32:LEU:HD13	1:A:34:ARG:HA	9	1.23
(1,578)	1:B:293:LEU:HD11	1:B:294:LYS:HB2	9	1.23
(1,578)	1:B:293:LEU:HD11	1:B:294:LYS:HB3	9	1.23
(1,578)	1:B:293:LEU:HD12	1:B:294:LYS:HB2	9	1.23
(1,578)	1:B:293:LEU:HD12	1:B:294:LYS:HB3	9	1.23
(1,578)	1:B:293:LEU:HD13	1:B:294:LYS:HB2	9	1.23
(1,578)	1:B:293:LEU:HD13	1:B:294:LYS:HB3	9	1.23
(1,578)	1:B:293:LEU:HD11	1:B:294:LYS:HB2	11	1.23
(1,578)	1:B:293:LEU:HD11	1:B:294:LYS:HB3	11	1.23
(1,578)	1:B:293:LEU:HD12	1:B:294:LYS:HB2	11	1.23
(1,578)	1:B:293:LEU:HD12	1:B:294:LYS:HB3	11	1.23
(1,578)	1:B:293:LEU:HD13	1:B:294:LYS:HB2	11	1.23
(1,578)	1:B:293:LEU:HD13	1:B:294:LYS:HB3	11	1.23
(1,577)	1:A:93:LEU:HD11	1:A:94:LYS:HB2	9	1.23
(1,577)	1:A:93:LEU:HD11	1:A:94:LYS:HB3	9	1.23
(1,577)	1:A:93:LEU:HD12	1:A:94:LYS:HB2	9	1.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,577)	1:A:93:LEU:HD12	1:A:94:LYS:HB3	9	1.23
(1,577)	1:A:93:LEU:HD13	1:A:94:LYS:HB2	9	1.23
(1,577)	1:A:93:LEU:HD13	1:A:94:LYS:HB3	9	1.23
(1,577)	1:A:93:LEU:HD11	1:A:94:LYS:HB2	11	1.23
(1,577)	1:A:93:LEU:HD11	1:A:94:LYS:HB3	11	1.23
(1,577)	1:A:93:LEU:HD12	1:A:94:LYS:HB2	11	1.23
(1,577)	1:A:93:LEU:HD12	1:A:94:LYS:HB3	11	1.23
(1,577)	1:A:93:LEU:HD13	1:A:94:LYS:HB2	11	1.23
(1,577)	1:A:93:LEU:HD13	1:A:94:LYS:HB3	11	1.23
(1,1268)	1:B:217:VAL:HG11	1:B:219:SER:H	7	1.23
(1,1268)	1:B:217:VAL:HG12	1:B:219:SER:H	7	1.23
(1,1268)	1:B:217:VAL:HG13	1:B:219:SER:H	7	1.23
(1,626)	1:B:250:GLN:HA	1:B:282:VAL:HG11	12	1.22
(1,626)	1:B:250:GLN:HA	1:B:282:VAL:HG12	12	1.22
(1,626)	1:B:250:GLN:HA	1:B:282:VAL:HG13	12	1.22
(1,578)	1:B:293:LEU:HD11	1:B:294:LYS:HB2	15	1.22
(1,578)	1:B:293:LEU:HD11	1:B:294:LYS:HB3	15	1.22
(1,578)	1:B:293:LEU:HD12	1:B:294:LYS:HB2	15	1.22
(1,578)	1:B:293:LEU:HD12	1:B:294:LYS:HB3	15	1.22
(1,578)	1:B:293:LEU:HD13	1:B:294:LYS:HB2	15	1.22
(1,578)	1:B:293:LEU:HD13	1:B:294:LYS:HB3	15	1.22
(1,577)	1:A:93:LEU:HD11	1:A:94:LYS:HB2	15	1.22
(1,577)	1:A:93:LEU:HD11	1:A:94:LYS:HB3	15	1.22
(1,577)	1:A:93:LEU:HD12	1:A:94:LYS:HB2	15	1.22
(1,577)	1:A:93:LEU:HD12	1:A:94:LYS:HB3	15	1.22
(1,577)	1:A:93:LEU:HD13	1:A:94:LYS:HB2	15	1.22
(1,577)	1:A:93:LEU:HD13	1:A:94:LYS:HB3	15	1.22
(1,550)	1:B:269:CYS:HB3	1:B:270:VAL:HB	10	1.22
(1,316)	1:B:232:LEU:HA	1:B:250:GLN:HB2	2	1.22
(1,932)	1:B:250:GLN:H	1:B:282:VAL:HG11	7	1.21
(1,932)	1:B:250:GLN:H	1:B:282:VAL:HG12	7	1.21
(1,932)	1:B:250:GLN:H	1:B:282:VAL:HG13	7	1.21
(1,577)	1:A:93:LEU:HD11	1:A:94:LYS:HB2	6	1.21
(1,577)	1:A:93:LEU:HD11	1:A:94:LYS:HB3	6	1.21
(1,577)	1:A:93:LEU:HD12	1:A:94:LYS:HB2	6	1.21
(1,577)	1:A:93:LEU:HD12	1:A:94:LYS:HB3	6	1.21
(1,577)	1:A:93:LEU:HD13	1:A:94:LYS:HB2	6	1.21
(1,577)	1:A:93:LEU:HD13	1:A:94:LYS:HB3	6	1.21
(1,498)	1:B:220:ASP:HB2	1:B:223:ARG:HD3	12	1.21
(1,34)	1:B:312:ASN:HA	1:B:315:LEU:HD21	2	1.21
(1,34)	1:B:312:ASN:HA	1:B:315:LEU:HD22	2	1.21
(1,34)	1:B:312:ASN:HA	1:B:315:LEU:HD23	2	1.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,627)	1:A:52:VAL:HG21	1:A:54:VAL:HA	16	1.2
(1,627)	1:A:52:VAL:HG22	1:A:54:VAL:HA	16	1.2
(1,627)	1:A:52:VAL:HG23	1:A:54:VAL:HA	16	1.2
(1,578)	1:B:293:LEU:HD11	1:B:294:LYS:HB2	5	1.2
(1,578)	1:B:293:LEU:HD11	1:B:294:LYS:HB3	5	1.2
(1,578)	1:B:293:LEU:HD12	1:B:294:LYS:HB2	5	1.2
(1,578)	1:B:293:LEU:HD12	1:B:294:LYS:HB3	5	1.2
(1,578)	1:B:293:LEU:HD13	1:B:294:LYS:HB2	5	1.2
(1,578)	1:B:293:LEU:HD13	1:B:294:LYS:HB3	5	1.2
(1,578)	1:B:293:LEU:HD11	1:B:294:LYS:HB2	6	1.2
(1,578)	1:B:293:LEU:HD11	1:B:294:LYS:HB3	6	1.2
(1,578)	1:B:293:LEU:HD12	1:B:294:LYS:HB2	6	1.2
(1,578)	1:B:293:LEU:HD12	1:B:294:LYS:HB3	6	1.2
(1,578)	1:B:293:LEU:HD13	1:B:294:LYS:HB2	6	1.2
(1,578)	1:B:293:LEU:HD13	1:B:294:LYS:HB3	6	1.2
(1,549)	1:B:220:ASP:HB2	1:B:221:PRO:HB2	15	1.2
(1,33)	1:A:112:ASN:HA	1:A:115:LEU:HD21	2	1.2
(1,33)	1:A:112:ASN:HA	1:A:115:LEU:HD22	2	1.2
(1,33)	1:A:112:ASN:HA	1:A:115:LEU:HD23	2	1.2
(1,30)	1:B:232:LEU:HD11	1:B:233:LEU:HA	5	1.2
(1,30)	1:B:232:LEU:HD12	1:B:233:LEU:HA	5	1.2
(1,30)	1:B:232:LEU:HD13	1:B:233:LEU:HA	5	1.2
(1,29)	1:A:32:LEU:HD11	1:A:33:LEU:HA	5	1.2
(1,29)	1:A:32:LEU:HD12	1:A:33:LEU:HA	5	1.2
(1,29)	1:A:32:LEU:HD13	1:A:33:LEU:HA	5	1.2
(1,97)	1:B:232:LEU:HD11	1:B:234:ARG:HA	10	1.19
(1,97)	1:B:232:LEU:HD12	1:B:234:ARG:HA	10	1.19
(1,97)	1:B:232:LEU:HD13	1:B:234:ARG:HA	10	1.19
(1,901)	1:A:103:ASN:H	1:A:125:VAL:HG21	1	1.19
(1,901)	1:A:103:ASN:H	1:A:125:VAL:HG22	1	1.19
(1,901)	1:A:103:ASN:H	1:A:125:VAL:HG23	1	1.19
(1,627)	1:A:52:VAL:HG21	1:A:54:VAL:HA	6	1.19
(1,627)	1:A:52:VAL:HG22	1:A:54:VAL:HA	6	1.19
(1,627)	1:A:52:VAL:HG23	1:A:54:VAL:HA	6	1.19
(1,577)	1:A:93:LEU:HD11	1:A:94:LYS:HB2	5	1.19
(1,577)	1:A:93:LEU:HD11	1:A:94:LYS:HB3	5	1.19
(1,577)	1:A:93:LEU:HD12	1:A:94:LYS:HB2	5	1.19
(1,577)	1:A:93:LEU:HD12	1:A:94:LYS:HB3	5	1.19
(1,577)	1:A:93:LEU:HD13	1:A:94:LYS:HB2	5	1.19
(1,577)	1:A:93:LEU:HD13	1:A:94:LYS:HB3	5	1.19
(1,1216)	1:B:231:SER:H	1:B:252:VAL:HG11	13	1.19
(1,1216)	1:B:231:SER:H	1:B:252:VAL:HG12	13	1.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1216)	1:B:231:SER:H	1:B:252:VAL:HG13	13	1.19
(1,461)	1:A:103:ASN:HA	1:A:105:ASP:HB2	12	1.18
(1,97)	1:B:232:LEU:HD11	1:B:234:ARG:HA	18	1.17
(1,97)	1:B:232:LEU:HD12	1:B:234:ARG:HA	18	1.17
(1,97)	1:B:232:LEU:HD13	1:B:234:ARG:HA	18	1.17
(1,930)	1:A:50:GLN:H	1:A:82:VAL:HG11	12	1.17
(1,930)	1:A:50:GLN:H	1:A:82:VAL:HG12	12	1.17
(1,930)	1:A:50:GLN:H	1:A:82:VAL:HG13	12	1.17
(1,315)	1:A:32:LEU:HA	1:A:50:GLN:HB2	4	1.17
(1,260)	1:B:228:PHE:HA	1:B:252:VAL:HB	12	1.17
(1,1282)	1:B:293:LEU:HD11	1:B:296:GLU:H	11	1.17
(1,1282)	1:B:293:LEU:HD12	1:B:296:GLU:H	11	1.17
(1,1282)	1:B:293:LEU:HD13	1:B:296:GLU:H	11	1.17
(1,1282)	1:B:293:LEU:HD11	1:B:296:GLU:H	12	1.17
(1,1282)	1:B:293:LEU:HD12	1:B:296:GLU:H	12	1.17
(1,1282)	1:B:293:LEU:HD13	1:B:296:GLU:H	12	1.17
(1,1281)	1:A:93:LEU:HD11	1:A:96:GLU:H	12	1.17
(1,1281)	1:A:93:LEU:HD12	1:A:96:GLU:H	12	1.17
(1,1281)	1:A:93:LEU:HD13	1:A:96:GLU:H	12	1.17
(1,514)	1:A:125:VAL:HB	1:B:205:PRO:HB2	6	1.16
(1,513)	1:A:5:PRO:HB2	1:B:325:VAL:HB	15	1.16
(1,298)	1:B:219:SER:HA	1:B:220:ASP:HB3	16	1.16
(1,280)	1:B:258:PRO:HB3	1:B:259:ALA:HA	1	1.16
(1,280)	1:B:258:PRO:HB3	1:B:259:ALA:HA	10	1.16
(1,280)	1:B:258:PRO:HB3	1:B:259:ALA:HA	16	1.16
(1,1281)	1:A:93:LEU:HD11	1:A:96:GLU:H	11	1.16
(1,1281)	1:A:93:LEU:HD12	1:A:96:GLU:H	11	1.16
(1,1281)	1:A:93:LEU:HD13	1:A:96:GLU:H	11	1.16
(1,679)	1:B:290:LEU:HD11	1:B:294:LYS:HG2	16	1.15
(1,679)	1:B:290:LEU:HD12	1:B:294:LYS:HG2	16	1.15
(1,679)	1:B:290:LEU:HD13	1:B:294:LYS:HG2	16	1.15
(1,609)	1:A:49:GLY:HA3	1:A:50:GLN:HB2	16	1.15
(1,549)	1:B:220:ASP:HB2	1:B:221:PRO:HB2	10	1.15
(1,547)	1:A:20:ASP:HB2	1:A:21:PRO:HB2	7	1.15
(1,462)	1:B:303:ASN:HA	1:B:305:ASP:HB2	11	1.15
(1,460)	1:B:302:ARG:HG3	1:B:305:ASP:HB2	7	1.15
(1,457)	1:A:102:ARG:HG3	1:A:105:ASP:HB2	7	1.15
(1,280)	1:B:258:PRO:HB3	1:B:259:ALA:HA	18	1.15
(1,280)	1:B:258:PRO:HB3	1:B:259:ALA:HA	20	1.15
(1,1267)	1:A:17:VAL:HG11	1:A:19:SER:H	8	1.15
(1,1267)	1:A:17:VAL:HG12	1:A:19:SER:H	8	1.15
(1,1267)	1:A:17:VAL:HG13	1:A:19:SER:H	8	1.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1216)	1:B:231:SER:H	1:B:252:VAL:HG11	18	1.15
(1,1216)	1:B:231:SER:H	1:B:252:VAL:HG12	18	1.15
(1,1216)	1:B:231:SER:H	1:B:252:VAL:HG13	18	1.15
(1,630)	1:B:252:VAL:HG21	1:B:279:ILE:HA	18	1.14
(1,630)	1:B:252:VAL:HG22	1:B:279:ILE:HA	18	1.14
(1,630)	1:B:252:VAL:HG23	1:B:279:ILE:HA	18	1.14
(1,610)	1:B:249:GLY:HA3	1:B:250:GLN:HB2	11	1.14
(1,587)	1:A:22:THR:H	1:A:23:ARG:HD3	12	1.14
(1,497)	1:A:20:ASP:HB2	1:A:23:ARG:HD3	8	1.14
(1,462)	1:B:303:ASN:HA	1:B:305:ASP:HB2	12	1.14
(1,280)	1:B:258:PRO:HB3	1:B:259:ALA:HA	7	1.14
(1,280)	1:B:258:PRO:HB3	1:B:259:ALA:HA	8	1.14
(1,280)	1:B:258:PRO:HB3	1:B:259:ALA:HA	13	1.14
(1,279)	1:A:58:PRO:HB3	1:A:59:ALA:HA	7	1.14
(1,279)	1:A:58:PRO:HB3	1:A:59:ALA:HA	10	1.14
(1,95)	1:A:32:LEU:HD11	1:A:34:ARG:HA	7	1.13
(1,95)	1:A:32:LEU:HD12	1:A:34:ARG:HA	7	1.13
(1,95)	1:A:32:LEU:HD13	1:A:34:ARG:HA	7	1.13
(1,930)	1:A:50:GLN:H	1:A:82:VAL:HG11	11	1.13
(1,930)	1:A:50:GLN:H	1:A:82:VAL:HG12	11	1.13
(1,930)	1:A:50:GLN:H	1:A:82:VAL:HG13	11	1.13
(1,610)	1:B:249:GLY:HA3	1:B:250:GLN:HB2	4	1.13
(1,549)	1:B:220:ASP:HB2	1:B:221:PRO:HB2	14	1.13
(1,498)	1:B:220:ASP:HB2	1:B:223:ARG:HD3	13	1.13
(1,280)	1:B:258:PRO:HB3	1:B:259:ALA:HA	3	1.13
(1,279)	1:A:58:PRO:HB3	1:A:59:ALA:HA	3	1.13
(1,279)	1:A:58:PRO:HB3	1:A:59:ALA:HA	9	1.13
(1,279)	1:A:58:PRO:HB3	1:A:59:ALA:HA	14	1.13
(1,279)	1:A:58:PRO:HB3	1:A:59:ALA:HA	15	1.13
(1,279)	1:A:58:PRO:HB3	1:A:59:ALA:HA	18	1.13
(1,279)	1:A:58:PRO:HB3	1:A:59:ALA:HA	20	1.13
(1,1311)	1:A:32:LEU:HD11	1:A:34:ARG:H	7	1.13
(1,1311)	1:A:32:LEU:HD12	1:A:34:ARG:H	7	1.13
(1,1311)	1:A:32:LEU:HD13	1:A:34:ARG:H	7	1.13
(1,1282)	1:B:293:LEU:HD11	1:B:296:GLU:H	5	1.13
(1,1282)	1:B:293:LEU:HD12	1:B:296:GLU:H	5	1.13
(1,1282)	1:B:293:LEU:HD13	1:B:296:GLU:H	5	1.13
(1,799)	1:A:112:ASN:H	1:A:115:LEU:HD21	12	1.12
(1,799)	1:A:112:ASN:H	1:A:115:LEU:HD22	12	1.12
(1,799)	1:A:112:ASN:H	1:A:115:LEU:HD23	12	1.12
(1,628)	1:A:52:VAL:HG21	1:A:79:ILE:HA	16	1.12
(1,628)	1:A:52:VAL:HG22	1:A:79:ILE:HA	16	1.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,628)	1:A:52:VAL:HG23	1:A:79:ILE:HA	16	1.12
(1,549)	1:B:220:ASP:HB2	1:B:221:PRO:HB2	16	1.12
(1,513)	1:A:5:PRO:HB2	1:B:325:VAL:HB	6	1.12
(1,461)	1:A:103:ASN:HA	1:A:105:ASP:HB2	11	1.12
(1,298)	1:B:219:SER:HA	1:B:220:ASP:HB3	7	1.12
(1,280)	1:B:258:PRO:HB3	1:B:259:ALA:HA	2	1.12
(1,280)	1:B:258:PRO:HB3	1:B:259:ALA:HA	9	1.12
(1,280)	1:B:258:PRO:HB3	1:B:259:ALA:HA	15	1.12
(1,279)	1:A:58:PRO:HB3	1:A:59:ALA:HA	1	1.12
(1,279)	1:A:58:PRO:HB3	1:A:59:ALA:HA	2	1.12
(1,1281)	1:A:93:LEU:HD11	1:A:96:GLU:H	5	1.12
(1,1281)	1:A:93:LEU:HD12	1:A:96:GLU:H	5	1.12
(1,1281)	1:A:93:LEU:HD13	1:A:96:GLU:H	5	1.12
(1,1267)	1:A:17:VAL:HG11	1:A:19:SER:H	16	1.12
(1,1267)	1:A:17:VAL:HG12	1:A:19:SER:H	16	1.12
(1,1267)	1:A:17:VAL:HG13	1:A:19:SER:H	16	1.12
(1,932)	1:B:250:GLN:H	1:B:282:VAL:HG11	2	1.11
(1,932)	1:B:250:GLN:H	1:B:282:VAL:HG12	2	1.11
(1,932)	1:B:250:GLN:H	1:B:282:VAL:HG13	2	1.11
(1,628)	1:A:52:VAL:HG21	1:A:79:ILE:HA	9	1.11
(1,628)	1:A:52:VAL:HG22	1:A:79:ILE:HA	9	1.11
(1,628)	1:A:52:VAL:HG23	1:A:79:ILE:HA	9	1.11
(1,628)	1:A:52:VAL:HG21	1:A:79:ILE:HA	15	1.11
(1,628)	1:A:52:VAL:HG22	1:A:79:ILE:HA	15	1.11
(1,628)	1:A:52:VAL:HG23	1:A:79:ILE:HA	15	1.11
(1,497)	1:A:20:ASP:HB2	1:A:23:ARG:HD3	13	1.11
(1,399)	1:A:102:ARG:HG2	1:A:124:ILE:HD11	1	1.11
(1,399)	1:A:102:ARG:HG2	1:A:124:ILE:HD12	1	1.11
(1,399)	1:A:102:ARG:HG2	1:A:124:ILE:HD13	1	1.11
(1,316)	1:B:232:LEU:HA	1:B:250:GLN:HB2	14	1.11
(1,280)	1:B:258:PRO:HB3	1:B:259:ALA:HA	14	1.11
(1,279)	1:A:58:PRO:HB3	1:A:59:ALA:HA	8	1.11
(1,1312)	1:B:232:LEU:HD11	1:B:234:ARG:H	8	1.11
(1,1312)	1:B:232:LEU:HD12	1:B:234:ARG:H	8	1.11
(1,1312)	1:B:232:LEU:HD13	1:B:234:ARG:H	8	1.11
(1,609)	1:A:49:GLY:HA3	1:A:50:GLN:HB2	1	1.1
(1,461)	1:A:103:ASN:HA	1:A:105:ASP:HB2	6	1.1
(1,461)	1:A:103:ASN:HA	1:A:105:ASP:HB2	18	1.1
(1,279)	1:A:58:PRO:HB3	1:A:59:ALA:HA	5	1.1
(1,61)	1:A:107:LEU:HB2	1:A:108:PHE:HA	8	1.09
(1,588)	1:B:222:THR:H	1:B:223:ARG:HD3	12	1.09
(1,524)	1:B:325:VAL:HB	1:B:326:SER:HA	17	1.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,523)	1:A:125:VAL:HB	1:A:126:SER:HA	1	1.09
(1,316)	1:B:232:LEU:HA	1:B:250:GLN:HB2	16	1.09
(1,279)	1:A:58:PRO:HB3	1:A:59:ALA:HA	13	1.09
(1,1216)	1:B:231:SER:H	1:B:252:VAL:HG11	11	1.09
(1,1216)	1:B:231:SER:H	1:B:252:VAL:HG12	11	1.09
(1,1216)	1:B:231:SER:H	1:B:252:VAL:HG13	11	1.09
(1,930)	1:A:50:GLN:H	1:A:82:VAL:HG11	2	1.08
(1,930)	1:A:50:GLN:H	1:A:82:VAL:HG12	2	1.08
(1,930)	1:A:50:GLN:H	1:A:82:VAL:HG13	2	1.08
(1,62)	1:B:307:LEU:HB2	1:B:308:PHE:HA	16	1.08
(1,498)	1:B:220:ASP:HB2	1:B:223:ARG:HD3	6	1.08
(1,932)	1:B:250:GLN:H	1:B:282:VAL:HG11	17	1.07
(1,932)	1:B:250:GLN:H	1:B:282:VAL:HG12	17	1.07
(1,932)	1:B:250:GLN:H	1:B:282:VAL:HG13	17	1.07
(1,800)	1:B:312:ASN:H	1:B:315:LEU:HD21	12	1.07
(1,800)	1:B:312:ASN:H	1:B:315:LEU:HD22	12	1.07
(1,800)	1:B:312:ASN:H	1:B:315:LEU:HD23	12	1.07
(1,62)	1:B:307:LEU:HB2	1:B:308:PHE:HA	8	1.07
(1,61)	1:A:107:LEU:HB2	1:A:108:PHE:HA	16	1.07
(1,609)	1:A:49:GLY:HA3	1:A:50:GLN:HB2	14	1.07
(1,514)	1:A:125:VAL:HB	1:B:205:PRO:HB2	13	1.07
(1,514)	1:A:125:VAL:HB	1:B:205:PRO:HB2	15	1.07
(1,513)	1:A:5:PRO:HB2	1:B:325:VAL:HB	4	1.07
(1,462)	1:B:303:ASN:HA	1:B:305:ASP:HB2	20	1.07
(1,280)	1:B:258:PRO:HB3	1:B:259:ALA:HA	5	1.07
(1,668)	1:B:288:GLU:HB2	1:B:289:ASN:HB2	1	1.06
(1,668)	1:B:288:GLU:HB2	1:B:289:ASN:HB3	1	1.06
(1,667)	1:A:88:GLU:HB2	1:A:89:ASN:HB2	12	1.06
(1,667)	1:A:88:GLU:HB2	1:A:89:ASN:HB3	12	1.06
(1,610)	1:B:249:GLY:HA3	1:B:250:GLN:HB2	1	1.06
(1,61)	1:A:107:LEU:HB2	1:A:108:PHE:HA	7	1.06
(1,547)	1:A:20:ASP:HB2	1:A:21:PRO:HB2	14	1.06
(1,462)	1:B:303:ASN:HA	1:B:305:ASP:HB2	18	1.06
(1,316)	1:B:232:LEU:HA	1:B:250:GLN:HB2	20	1.06
(1,315)	1:A:32:LEU:HA	1:A:50:GLN:HB2	5	1.06
(1,298)	1:B:219:SER:HA	1:B:220:ASP:HB3	8	1.06
(1,280)	1:B:258:PRO:HB3	1:B:259:ALA:HA	4	1.06
(1,1311)	1:A:32:LEU:HD11	1:A:34:ARG:H	8	1.06
(1,1311)	1:A:32:LEU:HD12	1:A:34:ARG:H	8	1.06
(1,1311)	1:A:32:LEU:HD13	1:A:34:ARG:H	8	1.06
(1,932)	1:B:250:GLN:H	1:B:282:VAL:HG11	6	1.05
(1,932)	1:B:250:GLN:H	1:B:282:VAL:HG12	6	1.05

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,932)	1:B:250:GLN:H	1:B:282:VAL:HG13	6	1.05
(1,62)	1:B:307:LEU:HB2	1:B:308:PHE:HA	7	1.05
(1,62)	1:B:307:LEU:HB2	1:B:308:PHE:HA	17	1.05
(1,61)	1:A:107:LEU:HB2	1:A:108:PHE:HA	17	1.05
(1,523)	1:A:125:VAL:HB	1:A:126:SER:HA	20	1.05
(1,513)	1:A:5:PRO:HB2	1:B:325:VAL:HB	1	1.05
(1,461)	1:A:103:ASN:HA	1:A:105:ASP:HB2	20	1.05
(1,279)	1:A:58:PRO:HB3	1:A:59:ALA:HA	4	1.05
(1,635)	1:A:125:VAL:HG21	1:B:205:PRO:HB2	8	1.04
(1,635)	1:A:125:VAL:HG22	1:B:205:PRO:HB2	8	1.04
(1,635)	1:A:125:VAL:HG23	1:B:205:PRO:HB2	8	1.04
(1,630)	1:B:252:VAL:HG21	1:B:279:ILE:HA	14	1.04
(1,630)	1:B:252:VAL:HG22	1:B:279:ILE:HA	14	1.04
(1,630)	1:B:252:VAL:HG23	1:B:279:ILE:HA	14	1.04
(1,609)	1:A:49:GLY:HA3	1:A:50:GLN:HB2	6	1.04
(1,609)	1:A:49:GLY:HA3	1:A:50:GLN:HB2	10	1.04
(1,609)	1:A:49:GLY:HA3	1:A:50:GLN:HB2	17	1.04
(1,497)	1:A:20:ASP:HB2	1:A:23:ARG:HD3	6	1.04
(1,1249)	1:A:70:VAL:HG11	1:A:72:MET:H	10	1.04
(1,1249)	1:A:70:VAL:HG12	1:A:72:MET:H	10	1.04
(1,1249)	1:A:70:VAL:HG13	1:A:72:MET:H	10	1.04
(1,1249)	1:A:70:VAL:HG11	1:A:72:MET:H	16	1.04
(1,1249)	1:A:70:VAL:HG12	1:A:72:MET:H	16	1.04
(1,1249)	1:A:70:VAL:HG13	1:A:72:MET:H	16	1.04
(1,62)	1:B:307:LEU:HB2	1:B:308:PHE:HA	1	1.03
(1,610)	1:B:249:GLY:HA3	1:B:250:GLN:HB2	5	1.03
(1,609)	1:A:49:GLY:HA3	1:A:50:GLN:HB2	11	1.03
(1,280)	1:B:258:PRO:HB3	1:B:259:ALA:HA	19	1.03
(1,224)	1:B:315:LEU:HD21	1:B:316:GLY:HA2	11	1.03
(1,224)	1:B:315:LEU:HD22	1:B:316:GLY:HA2	11	1.03
(1,224)	1:B:315:LEU:HD23	1:B:316:GLY:HA2	11	1.03
(1,633)	1:A:5:PRO:HB2	1:B:325:VAL:HG21	4	1.02
(1,633)	1:A:5:PRO:HB2	1:B:325:VAL:HG22	4	1.02
(1,633)	1:A:5:PRO:HB2	1:B:325:VAL:HG23	4	1.02
(1,628)	1:A:52:VAL:HG21	1:A:79:ILE:HA	10	1.02
(1,628)	1:A:52:VAL:HG22	1:A:79:ILE:HA	10	1.02
(1,628)	1:A:52:VAL:HG23	1:A:79:ILE:HA	10	1.02
(1,628)	1:A:52:VAL:HG21	1:A:79:ILE:HA	18	1.02
(1,628)	1:A:52:VAL:HG22	1:A:79:ILE:HA	18	1.02
(1,628)	1:A:52:VAL:HG23	1:A:79:ILE:HA	18	1.02
(1,610)	1:B:249:GLY:HA3	1:B:250:GLN:HB2	8	1.02
(1,610)	1:B:249:GLY:HA3	1:B:250:GLN:HB2	10	1.02

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,61)	1:A:107:LEU:HB2	1:A:108:PHE:HA	1	1.02
(1,901)	1:A:103:ASN:H	1:A:125:VAL:HG21	20	1.01
(1,901)	1:A:103:ASN:H	1:A:125:VAL:HG22	20	1.01
(1,901)	1:A:103:ASN:H	1:A:125:VAL:HG23	20	1.01
(1,668)	1:B:288:GLU:HB2	1:B:289:ASN:HB2	12	1.01
(1,668)	1:B:288:GLU:HB2	1:B:289:ASN:HB3	12	1.01
(1,630)	1:B:252:VAL:HG21	1:B:279:ILE:HA	4	1.01
(1,630)	1:B:252:VAL:HG22	1:B:279:ILE:HA	4	1.01
(1,630)	1:B:252:VAL:HG23	1:B:279:ILE:HA	4	1.01
(1,613)	1:A:20:ASP:HA	1:A:23:ARG:HB2	15	1.01
(1,584)	1:A:75:GLU:HB3	1:B:244:LEU:HD11	16	1.01
(1,584)	1:A:75:GLU:HB3	1:B:244:LEU:HD12	16	1.01
(1,584)	1:A:75:GLU:HB3	1:B:244:LEU:HD13	16	1.01
(1,482)	1:B:302:ARG:H	1:B:302:ARG:HD3	6	1.01
(1,680)	1:B:293:LEU:HD11	1:B:294:LYS:HG2	10	1.0
(1,680)	1:B:293:LEU:HD12	1:B:294:LYS:HG2	10	1.0
(1,680)	1:B:293:LEU:HD13	1:B:294:LYS:HG2	10	1.0
(1,610)	1:B:249:GLY:HA3	1:B:250:GLN:HB2	6	1.0
(1,547)	1:A:20:ASP:HB2	1:A:21:PRO:HB2	10	1.0
(1,513)	1:A:5:PRO:HB2	1:B:325:VAL:HB	5	1.0
(1,498)	1:B:220:ASP:HB2	1:B:223:ARG:HD3	11	1.0
(1,497)	1:A:20:ASP:HB2	1:A:23:ARG:HD3	12	1.0
(1,400)	1:B:302:ARG:HG2	1:B:324:ILE:HD11	1	1.0
(1,400)	1:B:302:ARG:HG2	1:B:324:ILE:HD12	1	1.0
(1,400)	1:B:302:ARG:HG2	1:B:324:ILE:HD13	1	1.0
(1,271)	1:A:20:ASP:HA	1:A:24:LEU:H	15	1.0
(1,609)	1:A:49:GLY:HA3	1:A:50:GLN:HB2	7	0.99
(1,1268)	1:B:217:VAL:HG11	1:B:219:SER:H	16	0.99
(1,1268)	1:B:217:VAL:HG12	1:B:219:SER:H	16	0.99
(1,1268)	1:B:217:VAL:HG13	1:B:219:SER:H	16	0.99
(1,780)	1:A:116:GLY:H	1:B:232:LEU:HD11	11	0.98
(1,780)	1:A:116:GLY:H	1:B:232:LEU:HD12	11	0.98
(1,780)	1:A:116:GLY:H	1:B:232:LEU:HD13	11	0.98
(1,718)	1:B:302:ARG:HG2	1:B:325:VAL:H	1	0.98
(1,610)	1:B:249:GLY:HA3	1:B:250:GLN:HB2	17	0.98
(1,609)	1:A:49:GLY:HA3	1:A:50:GLN:HB2	8	0.98
(1,481)	1:A:102:ARG:H	1:A:102:ARG:HD3	19	0.98
(1,297)	1:A:19:SER:HA	1:A:20:ASP:HB3	7	0.98
(1,279)	1:A:58:PRO:HB3	1:A:59:ALA:HA	17	0.98
(1,717)	1:A:102:ARG:HG2	1:A:125:VAL:H	1	0.97
(1,635)	1:A:125:VAL:HG21	1:B:205:PRO:HB2	6	0.97
(1,635)	1:A:125:VAL:HG22	1:B:205:PRO:HB2	6	0.97

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,635)	1:A:125:VAL:HG23	1:B:205:PRO:HB2	6	0.97
(1,554)	1:B:224:LEU:HB3	1:B:226:THR:HA	1	0.97
(1,513)	1:A:5:PRO:HB2	1:B:325:VAL:HB	20	0.97
(1,482)	1:B:302:ARG:H	1:B:302:ARG:HD3	10	0.97
(1,482)	1:B:302:ARG:H	1:B:302:ARG:HD3	19	0.97
(1,481)	1:A:102:ARG:H	1:A:102:ARG:HD3	10	0.97
(1,280)	1:B:258:PRO:HB3	1:B:259:ALA:HA	17	0.97
(1,279)	1:A:58:PRO:HB3	1:A:59:ALA:HA	19	0.97
(1,932)	1:B:250:GLN:H	1:B:282:VAL:HG11	1	0.96
(1,932)	1:B:250:GLN:H	1:B:282:VAL:HG12	1	0.96
(1,932)	1:B:250:GLN:H	1:B:282:VAL:HG13	1	0.96
(1,630)	1:B:252:VAL:HG21	1:B:279:ILE:HA	5	0.96
(1,630)	1:B:252:VAL:HG22	1:B:279:ILE:HA	5	0.96
(1,630)	1:B:252:VAL:HG23	1:B:279:ILE:HA	5	0.96
(1,610)	1:B:249:GLY:HA3	1:B:250:GLN:HB2	9	0.96
(1,610)	1:B:249:GLY:HA3	1:B:250:GLN:HB2	18	0.96
(1,609)	1:A:49:GLY:HA3	1:A:50:GLN:HB2	15	0.96
(1,514)	1:A:125:VAL:HB	1:B:205:PRO:HB2	3	0.96
(1,514)	1:A:125:VAL:HB	1:B:205:PRO:HB2	4	0.96
(1,514)	1:A:125:VAL:HB	1:B:205:PRO:HB2	5	0.96
(1,497)	1:A:20:ASP:HB2	1:A:23:ARG:HD3	11	0.96
(1,610)	1:B:249:GLY:HA3	1:B:250:GLN:HB2	15	0.95
(1,609)	1:A:49:GLY:HA3	1:A:50:GLN:HB2	9	0.95
(1,513)	1:A:5:PRO:HB2	1:B:325:VAL:HB	3	0.95
(1,315)	1:A:32:LEU:HA	1:A:50:GLN:HB2	20	0.95
(1,297)	1:A:19:SER:HA	1:A:20:ASP:HB3	8	0.95
(1,280)	1:B:258:PRO:HB3	1:B:259:ALA:HA	11	0.95
(1,279)	1:A:58:PRO:HB3	1:A:59:ALA:HA	16	0.95
(1,1151)	1:A:33:LEU:H	1:A:49:GLY:HA3	9	0.95
(1,610)	1:B:249:GLY:HA3	1:B:250:GLN:HB2	7	0.94
(1,609)	1:A:49:GLY:HA3	1:A:50:GLN:HB2	2	0.94
(1,609)	1:A:49:GLY:HA3	1:A:50:GLN:HB2	18	0.94
(1,513)	1:A:5:PRO:HB2	1:B:325:VAL:HB	11	0.94
(1,1066)	1:B:282:VAL:H	1:B:283:ILE:HG12	3	0.94
(1,930)	1:A:50:GLN:H	1:A:82:VAL:HG11	3	0.93
(1,930)	1:A:50:GLN:H	1:A:82:VAL:HG12	3	0.93
(1,930)	1:A:50:GLN:H	1:A:82:VAL:HG13	3	0.93
(1,635)	1:A:125:VAL:HG21	1:B:205:PRO:HB2	4	0.93
(1,635)	1:A:125:VAL:HG22	1:B:205:PRO:HB2	4	0.93
(1,635)	1:A:125:VAL:HG23	1:B:205:PRO:HB2	4	0.93
(1,635)	1:A:125:VAL:HG21	1:B:205:PRO:HB2	7	0.93
(1,635)	1:A:125:VAL:HG22	1:B:205:PRO:HB2	7	0.93

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,635)	1:A:125:VAL:HG23	1:B:205:PRO:HB2	7	0.93
(1,628)	1:A:52:VAL:HG21	1:A:79:ILE:HA	2	0.93
(1,628)	1:A:52:VAL:HG22	1:A:79:ILE:HA	2	0.93
(1,628)	1:A:52:VAL:HG23	1:A:79:ILE:HA	2	0.93
(1,628)	1:A:52:VAL:HG21	1:A:79:ILE:HA	4	0.93
(1,628)	1:A:52:VAL:HG22	1:A:79:ILE:HA	4	0.93
(1,628)	1:A:52:VAL:HG23	1:A:79:ILE:HA	4	0.93
(1,550)	1:B:269:CYS:HB3	1:B:270:VAL:HB	20	0.93
(1,548)	1:A:69:CYS:HB3	1:A:70:VAL:HB	8	0.93
(1,280)	1:B:258:PRO:HB3	1:B:259:ALA:HA	6	0.93
(1,279)	1:A:58:PRO:HB3	1:A:59:ALA:HA	6	0.93
(1,279)	1:A:58:PRO:HB3	1:A:59:ALA:HA	11	0.93
(1,498)	1:B:220:ASP:HB2	1:B:223:ARG:HD3	8	0.92
(1,1152)	1:B:233:LEU:H	1:B:249:GLY:HA3	9	0.92
(1,635)	1:A:125:VAL:HG21	1:B:205:PRO:HB2	13	0.91
(1,635)	1:A:125:VAL:HG22	1:B:205:PRO:HB2	13	0.91
(1,635)	1:A:125:VAL:HG23	1:B:205:PRO:HB2	13	0.91
(1,635)	1:A:125:VAL:HG21	1:B:205:PRO:HB2	19	0.91
(1,635)	1:A:125:VAL:HG22	1:B:205:PRO:HB2	19	0.91
(1,635)	1:A:125:VAL:HG23	1:B:205:PRO:HB2	19	0.91
(1,609)	1:A:49:GLY:HA3	1:A:50:GLN:HB2	20	0.91
(1,279)	1:A:58:PRO:HB3	1:A:59:ALA:HA	12	0.91
(1,657)	1:A:93:LEU:HD11	1:A:94:LYS:HG3	16	0.9
(1,657)	1:A:93:LEU:HD12	1:A:94:LYS:HG3	16	0.9
(1,657)	1:A:93:LEU:HD13	1:A:94:LYS:HG3	16	0.9
(1,635)	1:A:125:VAL:HG21	1:B:205:PRO:HB2	3	0.9
(1,635)	1:A:125:VAL:HG22	1:B:205:PRO:HB2	3	0.9
(1,635)	1:A:125:VAL:HG23	1:B:205:PRO:HB2	3	0.9
(1,633)	1:A:5:PRO:HB2	1:B:325:VAL:HG21	19	0.9
(1,633)	1:A:5:PRO:HB2	1:B:325:VAL:HG22	19	0.9
(1,633)	1:A:5:PRO:HB2	1:B:325:VAL:HG23	19	0.9
(1,633)	1:A:5:PRO:HB2	1:B:325:VAL:HG21	20	0.9
(1,633)	1:A:5:PRO:HB2	1:B:325:VAL:HG22	20	0.9
(1,633)	1:A:5:PRO:HB2	1:B:325:VAL:HG23	20	0.9
(1,628)	1:A:52:VAL:HG21	1:A:79:ILE:HA	5	0.9
(1,628)	1:A:52:VAL:HG22	1:A:79:ILE:HA	5	0.9
(1,628)	1:A:52:VAL:HG23	1:A:79:ILE:HA	5	0.9
(1,553)	1:A:24:LEU:HB3	1:A:26:THR:HA	10	0.9
(1,513)	1:A:5:PRO:HB2	1:B:325:VAL:HB	13	0.9
(1,461)	1:A:103:ASN:HA	1:A:105:ASP:HB2	17	0.9
(1,1282)	1:B:293:LEU:HD11	1:B:296:GLU:H	6	0.9
(1,1282)	1:B:293:LEU:HD12	1:B:296:GLU:H	6	0.9

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1282)	1:B:293:LEU:HD13	1:B:296:GLU:H	6	0.9
(1,635)	1:A:125:VAL:HG21	1:B:205:PRO:HB2	17	0.89
(1,635)	1:A:125:VAL:HG22	1:B:205:PRO:HB2	17	0.89
(1,635)	1:A:125:VAL:HG23	1:B:205:PRO:HB2	17	0.89
(1,633)	1:A:5:PRO:HB2	1:B:325:VAL:HG21	3	0.89
(1,633)	1:A:5:PRO:HB2	1:B:325:VAL:HG22	3	0.89
(1,633)	1:A:5:PRO:HB2	1:B:325:VAL:HG23	3	0.89
(1,61)	1:A:107:LEU:HB2	1:A:108:PHE:HA	20	0.89
(1,514)	1:A:125:VAL:HB	1:B:205:PRO:HB2	17	0.89
(1,514)	1:A:125:VAL:HB	1:B:205:PRO:HB2	19	0.89
(1,481)	1:A:102:ARG:H	1:A:102:ARG:HD3	11	0.89
(1,461)	1:A:103:ASN:HA	1:A:105:ASP:HB2	19	0.89
(1,457)	1:A:102:ARG:HG3	1:A:105:ASP:HB2	12	0.89
(1,280)	1:B:258:PRO:HB3	1:B:259:ALA:HA	12	0.89
(1,610)	1:B:249:GLY:HA3	1:B:250:GLN:HB2	3	0.88
(1,513)	1:A:5:PRO:HB2	1:B:325:VAL:HB	19	0.88
(1,1311)	1:A:32:LEU:HD11	1:A:34:ARG:H	11	0.88
(1,1311)	1:A:32:LEU:HD12	1:A:34:ARG:H	11	0.88
(1,1311)	1:A:32:LEU:HD13	1:A:34:ARG:H	11	0.88
(1,1268)	1:B:217:VAL:HG11	1:B:219:SER:H	17	0.88
(1,1268)	1:B:217:VAL:HG12	1:B:219:SER:H	17	0.88
(1,1268)	1:B:217:VAL:HG13	1:B:219:SER:H	17	0.88
(1,1216)	1:B:231:SER:H	1:B:252:VAL:HG11	12	0.88
(1,1216)	1:B:231:SER:H	1:B:252:VAL:HG12	12	0.88
(1,1216)	1:B:231:SER:H	1:B:252:VAL:HG13	12	0.88
(1,679)	1:B:290:LEU:HD11	1:B:294:LYS:HG2	13	0.87
(1,679)	1:B:290:LEU:HD12	1:B:294:LYS:HG2	13	0.87
(1,679)	1:B:290:LEU:HD13	1:B:294:LYS:HG2	13	0.87
(1,633)	1:A:5:PRO:HB2	1:B:325:VAL:HG21	8	0.87
(1,633)	1:A:5:PRO:HB2	1:B:325:VAL:HG22	8	0.87
(1,633)	1:A:5:PRO:HB2	1:B:325:VAL:HG23	8	0.87
(1,633)	1:A:5:PRO:HB2	1:B:325:VAL:HG21	11	0.87
(1,633)	1:A:5:PRO:HB2	1:B:325:VAL:HG22	11	0.87
(1,633)	1:A:5:PRO:HB2	1:B:325:VAL:HG23	11	0.87
(1,610)	1:B:249:GLY:HA3	1:B:250:GLN:HB2	19	0.87
(1,61)	1:A:107:LEU:HB2	1:A:108:PHE:HA	6	0.87
(1,609)	1:A:49:GLY:HA3	1:A:50:GLN:HB2	3	0.87
(1,553)	1:A:24:LEU:HB3	1:A:26:THR:HA	1	0.87
(1,498)	1:B:220:ASP:HB2	1:B:223:ARG:HD3	9	0.87
(1,498)	1:B:220:ASP:HB2	1:B:223:ARG:HD3	15	0.87
(1,482)	1:B:302:ARG:H	1:B:302:ARG:HD3	11	0.87
(1,29)	1:A:32:LEU:HD11	1:A:33:LEU:HA	20	0.87

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,29)	1:A:32:LEU:HD12	1:A:33:LEU:HA	20	0.87
(1,29)	1:A:32:LEU:HD13	1:A:33:LEU:HA	20	0.87
(1,1065)	1:A:82:VAL:H	1:A:83:ILE:HG12	3	0.87
(1,668)	1:B:288:GLU:HB2	1:B:289:ASN:HB2	19	0.86
(1,668)	1:B:288:GLU:HB2	1:B:289:ASN:HB3	19	0.86
(1,667)	1:A:88:GLU:HB2	1:A:89:ASN:HB2	19	0.86
(1,667)	1:A:88:GLU:HB2	1:A:89:ASN:HB3	19	0.86
(1,633)	1:A:5:PRO:HB2	1:B:325:VAL:HG21	6	0.86
(1,633)	1:A:5:PRO:HB2	1:B:325:VAL:HG22	6	0.86
(1,633)	1:A:5:PRO:HB2	1:B:325:VAL:HG23	6	0.86
(1,62)	1:B:307:LEU:HB2	1:B:308:PHE:HA	6	0.86
(1,513)	1:A:5:PRO:HB2	1:B:325:VAL:HB	12	0.86
(1,497)	1:A:20:ASP:HB2	1:A:23:ARG:HD3	9	0.86
(1,326)	1:A:5:PRO:HB3	1:A:6:MET:HA	8	0.86
(1,166)	1:B:244:LEU:HD11	1:B:286:SER:HA	10	0.86
(1,166)	1:B:244:LEU:HD12	1:B:286:SER:HA	10	0.86
(1,166)	1:B:244:LEU:HD13	1:B:286:SER:HA	10	0.86
(1,1107)	1:A:44:LEU:HD11	1:B:275:GLU:H	15	0.86
(1,1107)	1:A:44:LEU:HD12	1:B:275:GLU:H	15	0.86
(1,1107)	1:A:44:LEU:HD13	1:B:275:GLU:H	15	0.86
(1,582)	1:A:44:LEU:HD11	1:B:275:GLU:HB3	16	0.85
(1,582)	1:A:44:LEU:HD12	1:B:275:GLU:HB3	16	0.85
(1,582)	1:A:44:LEU:HD13	1:B:275:GLU:HB3	16	0.85
(1,514)	1:A:125:VAL:HB	1:B:205:PRO:HB2	11	0.85
(1,316)	1:B:232:LEU:HA	1:B:250:GLN:HB2	15	0.85
(1,164)	1:A:44:LEU:HD11	1:A:86:SER:HA	10	0.85
(1,164)	1:A:44:LEU:HD12	1:A:86:SER:HA	10	0.85
(1,164)	1:A:44:LEU:HD13	1:A:86:SER:HA	10	0.85
(1,1108)	1:A:75:GLU:H	1:B:244:LEU:HD11	5	0.85
(1,1108)	1:A:75:GLU:H	1:B:244:LEU:HD12	5	0.85
(1,1108)	1:A:75:GLU:H	1:B:244:LEU:HD13	5	0.85
(1,1107)	1:A:44:LEU:HD11	1:B:275:GLU:H	17	0.85
(1,1107)	1:A:44:LEU:HD12	1:B:275:GLU:H	17	0.85
(1,1107)	1:A:44:LEU:HD13	1:B:275:GLU:H	17	0.85
(1,633)	1:A:5:PRO:HB2	1:B:325:VAL:HG21	5	0.84
(1,633)	1:A:5:PRO:HB2	1:B:325:VAL:HG22	5	0.84
(1,633)	1:A:5:PRO:HB2	1:B:325:VAL:HG23	5	0.84
(1,62)	1:B:307:LEU:HB2	1:B:308:PHE:HA	20	0.84
(1,513)	1:A:5:PRO:HB2	1:B:325:VAL:HB	14	0.84
(1,460)	1:B:302:ARG:HG3	1:B:305:ASP:HB2	12	0.84
(1,326)	1:A:5:PRO:HB3	1:A:6:MET:HA	7	0.84
(1,1281)	1:A:93:LEU:HD11	1:A:96:GLU:H	16	0.84

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1281)	1:A:93:LEU:HD12	1:A:96:GLU:H	16	0.84
(1,1281)	1:A:93:LEU:HD13	1:A:96:GLU:H	16	0.84
(1,583)	1:A:73:PRO:HB3	1:B:244:LEU:HD11	20	0.83
(1,583)	1:A:73:PRO:HB3	1:B:244:LEU:HD12	20	0.83
(1,583)	1:A:73:PRO:HB3	1:B:244:LEU:HD13	20	0.83
(1,328)	1:B:205:PRO:HB3	1:B:206:MET:HA	17	0.83
(1,326)	1:A:5:PRO:HB3	1:A:6:MET:HA	17	0.83
(1,315)	1:A:32:LEU:HA	1:A:50:GLN:HB2	19	0.83
(1,1249)	1:A:70:VAL:HG11	1:A:72:MET:H	4	0.83
(1,1249)	1:A:70:VAL:HG12	1:A:72:MET:H	4	0.83
(1,1249)	1:A:70:VAL:HG13	1:A:72:MET:H	4	0.83
(1,1108)	1:A:75:GLU:H	1:B:244:LEU:HD11	17	0.83
(1,1108)	1:A:75:GLU:H	1:B:244:LEU:HD12	17	0.83
(1,1108)	1:A:75:GLU:H	1:B:244:LEU:HD13	17	0.83
(1,462)	1:B:303:ASN:HA	1:B:305:ASP:HB2	19	0.82
(1,315)	1:A:32:LEU:HA	1:A:50:GLN:HB2	2	0.82
(1,1312)	1:B:232:LEU:HD11	1:B:234:ARG:H	11	0.82
(1,1312)	1:B:232:LEU:HD12	1:B:234:ARG:H	11	0.82
(1,1312)	1:B:232:LEU:HD13	1:B:234:ARG:H	11	0.82
(1,1267)	1:A:17:VAL:HG11	1:A:19:SER:H	9	0.82
(1,1267)	1:A:17:VAL:HG12	1:A:19:SER:H	9	0.82
(1,1267)	1:A:17:VAL:HG13	1:A:19:SER:H	9	0.82
(1,800)	1:B:312:ASN:H	1:B:315:LEU:HD21	11	0.81
(1,800)	1:B:312:ASN:H	1:B:315:LEU:HD22	11	0.81
(1,800)	1:B:312:ASN:H	1:B:315:LEU:HD23	11	0.81
(1,635)	1:A:125:VAL:HG21	1:B:205:PRO:HB2	11	0.81
(1,635)	1:A:125:VAL:HG22	1:B:205:PRO:HB2	11	0.81
(1,635)	1:A:125:VAL:HG23	1:B:205:PRO:HB2	11	0.81
(1,633)	1:A:5:PRO:HB2	1:B:325:VAL:HG21	7	0.81
(1,633)	1:A:5:PRO:HB2	1:B:325:VAL:HG22	7	0.81
(1,633)	1:A:5:PRO:HB2	1:B:325:VAL:HG23	7	0.81
(1,482)	1:B:302:ARG:H	1:B:302:ARG:HD3	5	0.81
(1,481)	1:A:102:ARG:H	1:A:102:ARG:HD3	5	0.81
(1,328)	1:B:205:PRO:HB3	1:B:206:MET:HA	7	0.81
(1,328)	1:B:205:PRO:HB3	1:B:206:MET:HA	13	0.81
(1,328)	1:B:205:PRO:HB3	1:B:206:MET:HA	20	0.81
(1,326)	1:A:5:PRO:HB3	1:A:6:MET:HA	4	0.81
(1,326)	1:A:5:PRO:HB3	1:A:6:MET:HA	13	0.81
(1,297)	1:A:19:SER:HA	1:A:20:ASP:HB3	14	0.81
(1,778)	1:A:32:LEU:HD11	1:B:316:GLY:H	11	0.8
(1,778)	1:A:32:LEU:HD12	1:B:316:GLY:H	11	0.8
(1,778)	1:A:32:LEU:HD13	1:B:316:GLY:H	11	0.8

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,657)	1:A:93:LEU:HD11	1:A:94:LYS:HG3	9	0.8
(1,657)	1:A:93:LEU:HD12	1:A:94:LYS:HG3	9	0.8
(1,657)	1:A:93:LEU:HD13	1:A:94:LYS:HG3	9	0.8
(1,633)	1:A:5:PRO:HB2	1:B:325:VAL:HG21	14	0.8
(1,633)	1:A:5:PRO:HB2	1:B:325:VAL:HG22	14	0.8
(1,633)	1:A:5:PRO:HB2	1:B:325:VAL:HG23	14	0.8
(1,633)	1:A:5:PRO:HB2	1:B:325:VAL:HG21	15	0.8
(1,633)	1:A:5:PRO:HB2	1:B:325:VAL:HG22	15	0.8
(1,633)	1:A:5:PRO:HB2	1:B:325:VAL:HG23	15	0.8
(1,630)	1:B:252:VAL:HG21	1:B:279:ILE:HA	2	0.8
(1,630)	1:B:252:VAL:HG22	1:B:279:ILE:HA	2	0.8
(1,630)	1:B:252:VAL:HG23	1:B:279:ILE:HA	2	0.8
(1,62)	1:B:307:LEU:HB2	1:B:308:PHE:HA	4	0.8
(1,61)	1:A:107:LEU:HB2	1:A:108:PHE:HA	4	0.8
(1,609)	1:A:49:GLY:HA3	1:A:50:GLN:HB2	19	0.8
(1,498)	1:B:220:ASP:HB2	1:B:223:ARG:HD3	17	0.8
(1,328)	1:B:205:PRO:HB3	1:B:206:MET:HA	8	0.8
(1,328)	1:B:205:PRO:HB3	1:B:206:MET:HA	9	0.8
(1,326)	1:A:5:PRO:HB3	1:A:6:MET:HA	5	0.8
(1,1281)	1:A:93:LEU:HD11	1:A:96:GLU:H	9	0.8
(1,1281)	1:A:93:LEU:HD12	1:A:96:GLU:H	9	0.8
(1,1281)	1:A:93:LEU:HD13	1:A:96:GLU:H	9	0.8
(1,1108)	1:A:75:GLU:H	1:B:244:LEU:HD11	15	0.8
(1,1108)	1:A:75:GLU:H	1:B:244:LEU:HD12	15	0.8
(1,1108)	1:A:75:GLU:H	1:B:244:LEU:HD13	15	0.8
(1,658)	1:B:293:LEU:HD11	1:B:294:LYS:HG3	6	0.79
(1,658)	1:B:293:LEU:HD12	1:B:294:LYS:HG3	6	0.79
(1,658)	1:B:293:LEU:HD13	1:B:294:LYS:HG3	6	0.79
(1,633)	1:A:5:PRO:HB2	1:B:325:VAL:HG21	13	0.79
(1,633)	1:A:5:PRO:HB2	1:B:325:VAL:HG22	13	0.79
(1,633)	1:A:5:PRO:HB2	1:B:325:VAL:HG23	13	0.79
(1,628)	1:A:52:VAL:HG21	1:A:79:ILE:HA	3	0.79
(1,628)	1:A:52:VAL:HG22	1:A:79:ILE:HA	3	0.79
(1,628)	1:A:52:VAL:HG23	1:A:79:ILE:HA	3	0.79
(1,553)	1:A:24:LEU:HB3	1:A:26:THR:HA	19	0.79
(1,328)	1:B:205:PRO:HB3	1:B:206:MET:HA	6	0.79
(1,326)	1:A:5:PRO:HB3	1:A:6:MET:HA	9	0.79
(1,587)	1:A:22:THR:H	1:A:23:ARG:HD3	17	0.78
(1,579)	1:A:125:VAL:HG11	1:B:205:PRO:HB2	20	0.78
(1,579)	1:A:125:VAL:HG12	1:B:205:PRO:HB2	20	0.78
(1,579)	1:A:125:VAL:HG13	1:B:205:PRO:HB2	20	0.78
(1,326)	1:A:5:PRO:HB3	1:A:6:MET:HA	6	0.78

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,165)	1:B:247:VAL:HG21	1:B:286:SER:HA	2	0.78
(1,165)	1:B:247:VAL:HG22	1:B:286:SER:HA	2	0.78
(1,165)	1:B:247:VAL:HG23	1:B:286:SER:HA	2	0.78
(1,1268)	1:B:217:VAL:HG11	1:B:219:SER:H	4	0.78
(1,1268)	1:B:217:VAL:HG12	1:B:219:SER:H	4	0.78
(1,1268)	1:B:217:VAL:HG13	1:B:219:SER:H	4	0.78
(1,1268)	1:B:217:VAL:HG11	1:B:219:SER:H	14	0.78
(1,1268)	1:B:217:VAL:HG12	1:B:219:SER:H	14	0.78
(1,1268)	1:B:217:VAL:HG13	1:B:219:SER:H	14	0.78
(1,668)	1:B:288:GLU:HB2	1:B:289:ASN:HB2	10	0.77
(1,668)	1:B:288:GLU:HB2	1:B:289:ASN:HB3	10	0.77
(1,667)	1:A:88:GLU:HB2	1:A:89:ASN:HB2	10	0.77
(1,667)	1:A:88:GLU:HB2	1:A:89:ASN:HB3	10	0.77
(1,658)	1:B:293:LEU:HD11	1:B:294:LYS:HG3	9	0.77
(1,658)	1:B:293:LEU:HD12	1:B:294:LYS:HG3	9	0.77
(1,658)	1:B:293:LEU:HD13	1:B:294:LYS:HG3	9	0.77
(1,63)	1:A:107:LEU:HD11	1:A:108:PHE:HA	19	0.77
(1,63)	1:A:107:LEU:HD12	1:A:108:PHE:HA	19	0.77
(1,63)	1:A:107:LEU:HD13	1:A:108:PHE:HA	19	0.77
(1,62)	1:B:307:LEU:HB2	1:B:308:PHE:HA	19	0.77
(1,481)	1:A:102:ARG:H	1:A:102:ARG:HD3	3	0.77
(1,461)	1:A:103:ASN:HA	1:A:105:ASP:HB2	2	0.77
(1,328)	1:B:205:PRO:HB3	1:B:206:MET:HA	4	0.77
(1,326)	1:A:5:PRO:HB3	1:A:6:MET:HA	20	0.77
(1,298)	1:B:219:SER:HA	1:B:220:ASP:HB3	14	0.77
(1,153)	1:A:88:GLU:HB2	1:A:89:ASN:HA	1	0.77
(1,1107)	1:A:44:LEU:HD11	1:B:275:GLU:H	5	0.77
(1,1107)	1:A:44:LEU:HD12	1:B:275:GLU:H	5	0.77
(1,1107)	1:A:44:LEU:HD13	1:B:275:GLU:H	5	0.77
(1,1066)	1:B:282:VAL:H	1:B:283:ILE:HG12	14	0.77
(1,633)	1:A:5:PRO:HB2	1:B:325:VAL:HG21	12	0.76
(1,633)	1:A:5:PRO:HB2	1:B:325:VAL:HG22	12	0.76
(1,633)	1:A:5:PRO:HB2	1:B:325:VAL:HG23	12	0.76
(1,62)	1:B:307:LEU:HB2	1:B:308:PHE:HA	15	0.76
(1,62)	1:B:307:LEU:HB2	1:B:308:PHE:HA	18	0.76
(1,61)	1:A:107:LEU:HB2	1:A:108:PHE:HA	15	0.76
(1,61)	1:A:107:LEU:HB2	1:A:108:PHE:HA	18	0.76
(1,61)	1:A:107:LEU:HB2	1:A:108:PHE:HA	19	0.76
(1,482)	1:B:302:ARG:H	1:B:302:ARG:HD3	3	0.76
(1,1268)	1:B:217:VAL:HG11	1:B:219:SER:H	1	0.76
(1,1268)	1:B:217:VAL:HG12	1:B:219:SER:H	1	0.76
(1,1268)	1:B:217:VAL:HG13	1:B:219:SER:H	1	0.76

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1214)	1:A:31:SER:H	1:A:52:VAL:HG11	19	0.76
(1,1214)	1:A:31:SER:H	1:A:52:VAL:HG12	19	0.76
(1,1214)	1:A:31:SER:H	1:A:52:VAL:HG13	19	0.76
(1,1066)	1:B:282:VAL:H	1:B:283:ILE:HG12	7	0.76
(1,667)	1:A:88:GLU:HB2	1:A:89:ASN:HB2	14	0.75
(1,667)	1:A:88:GLU:HB2	1:A:89:ASN:HB3	14	0.75
(1,64)	1:B:307:LEU:HD11	1:B:308:PHE:HA	19	0.75
(1,64)	1:B:307:LEU:HD12	1:B:308:PHE:HA	19	0.75
(1,64)	1:B:307:LEU:HD13	1:B:308:PHE:HA	19	0.75
(1,581)	1:A:44:LEU:HD11	1:B:273:PRO:HB3	10	0.75
(1,581)	1:A:44:LEU:HD12	1:B:273:PRO:HB3	10	0.75
(1,581)	1:A:44:LEU:HD13	1:B:273:PRO:HB3	10	0.75
(1,550)	1:B:269:CYS:HB3	1:B:270:VAL:HB	7	0.75
(1,328)	1:B:205:PRO:HB3	1:B:206:MET:HA	19	0.75
(1,153)	1:A:88:GLU:HB2	1:A:89:ASN:HA	10	0.75
(1,717)	1:A:102:ARG:HG2	1:A:125:VAL:H	6	0.74
(1,668)	1:B:288:GLU:HB2	1:B:289:ASN:HB2	4	0.74
(1,668)	1:B:288:GLU:HB2	1:B:289:ASN:HB3	4	0.74
(1,667)	1:A:88:GLU:HB2	1:A:89:ASN:HB2	4	0.74
(1,667)	1:A:88:GLU:HB2	1:A:89:ASN:HB3	4	0.74
(1,635)	1:A:125:VAL:HG21	1:B:205:PRO:HB2	15	0.74
(1,635)	1:A:125:VAL:HG22	1:B:205:PRO:HB2	15	0.74
(1,635)	1:A:125:VAL:HG23	1:B:205:PRO:HB2	15	0.74
(1,514)	1:A:125:VAL:HB	1:B:205:PRO:HB2	10	0.74
(1,154)	1:B:288:GLU:HB2	1:B:289:ASN:HA	10	0.74
(1,1282)	1:B:293:LEU:HD11	1:B:296:GLU:H	10	0.74
(1,1282)	1:B:293:LEU:HD12	1:B:296:GLU:H	10	0.74
(1,1282)	1:B:293:LEU:HD13	1:B:296:GLU:H	10	0.74
(1,1267)	1:A:17:VAL:HG11	1:A:19:SER:H	7	0.74
(1,1267)	1:A:17:VAL:HG12	1:A:19:SER:H	7	0.74
(1,1267)	1:A:17:VAL:HG13	1:A:19:SER:H	7	0.74
(1,1250)	1:B:270:VAL:HG11	1:B:272:MET:H	8	0.74
(1,1250)	1:B:270:VAL:HG12	1:B:272:MET:H	8	0.74
(1,1250)	1:B:270:VAL:HG13	1:B:272:MET:H	8	0.74
(1,668)	1:B:288:GLU:HB2	1:B:289:ASN:HB2	14	0.73
(1,668)	1:B:288:GLU:HB2	1:B:289:ASN:HB3	14	0.73
(1,635)	1:A:125:VAL:HG21	1:B:205:PRO:HB2	2	0.73
(1,635)	1:A:125:VAL:HG22	1:B:205:PRO:HB2	2	0.73
(1,635)	1:A:125:VAL:HG23	1:B:205:PRO:HB2	2	0.73
(1,61)	1:A:107:LEU:HB2	1:A:108:PHE:HA	14	0.73
(1,328)	1:B:205:PRO:HB3	1:B:206:MET:HA	5	0.73
(1,328)	1:B:205:PRO:HB3	1:B:206:MET:HA	10	0.73

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,326)	1:A:5:PRO:HB3	1:A:6:MET:HA	10	0.73
(1,326)	1:A:5:PRO:HB3	1:A:6:MET:HA	19	0.73
(1,298)	1:B:219:SER:HA	1:B:220:ASP:HB3	10	0.73
(1,297)	1:A:19:SER:HA	1:A:20:ASP:HB3	10	0.73
(1,154)	1:B:288:GLU:HB2	1:B:289:ASN:HA	1	0.73
(1,154)	1:B:288:GLU:HB2	1:B:289:ASN:HA	4	0.73
(1,154)	1:B:288:GLU:HB2	1:B:289:ASN:HA	12	0.73
(1,153)	1:A:88:GLU:HB2	1:A:89:ASN:HA	12	0.73
(1,1312)	1:B:232:LEU:HD11	1:B:234:ARG:H	19	0.73
(1,1312)	1:B:232:LEU:HD12	1:B:234:ARG:H	19	0.73
(1,1312)	1:B:232:LEU:HD13	1:B:234:ARG:H	19	0.73
(1,635)	1:A:125:VAL:HG21	1:B:205:PRO:HB2	10	0.72
(1,635)	1:A:125:VAL:HG22	1:B:205:PRO:HB2	10	0.72
(1,635)	1:A:125:VAL:HG23	1:B:205:PRO:HB2	10	0.72
(1,62)	1:B:307:LEU:HB2	1:B:308:PHE:HA	14	0.72
(1,61)	1:A:107:LEU:HB2	1:A:108:PHE:HA	2	0.72
(1,578)	1:B:293:LEU:HD11	1:B:294:LYS:HB2	10	0.72
(1,578)	1:B:293:LEU:HD11	1:B:294:LYS:HB3	10	0.72
(1,578)	1:B:293:LEU:HD12	1:B:294:LYS:HB2	10	0.72
(1,578)	1:B:293:LEU:HD12	1:B:294:LYS:HB3	10	0.72
(1,578)	1:B:293:LEU:HD13	1:B:294:LYS:HB2	10	0.72
(1,578)	1:B:293:LEU:HD13	1:B:294:LYS:HB3	10	0.72
(1,153)	1:A:88:GLU:HB2	1:A:89:ASN:HA	4	0.72
(1,1282)	1:B:293:LEU:HD11	1:B:296:GLU:H	9	0.72
(1,1282)	1:B:293:LEU:HD12	1:B:296:GLU:H	9	0.72
(1,1282)	1:B:293:LEU:HD13	1:B:296:GLU:H	9	0.72
(1,1281)	1:A:93:LEU:HD11	1:A:96:GLU:H	15	0.72
(1,1281)	1:A:93:LEU:HD12	1:A:96:GLU:H	15	0.72
(1,1281)	1:A:93:LEU:HD13	1:A:96:GLU:H	15	0.72
(1,679)	1:B:290:LEU:HD11	1:B:294:LYS:HG2	11	0.71
(1,679)	1:B:290:LEU:HD12	1:B:294:LYS:HG2	11	0.71
(1,679)	1:B:290:LEU:HD13	1:B:294:LYS:HG2	11	0.71
(1,677)	1:A:90:LEU:HD11	1:A:94:LYS:HG2	11	0.71
(1,677)	1:A:90:LEU:HD12	1:A:94:LYS:HG2	11	0.71
(1,677)	1:A:90:LEU:HD13	1:A:94:LYS:HG2	11	0.71
(1,62)	1:B:307:LEU:HB2	1:B:308:PHE:HA	2	0.71
(1,579)	1:A:125:VAL:HG11	1:B:205:PRO:HB2	1	0.71
(1,579)	1:A:125:VAL:HG12	1:B:205:PRO:HB2	1	0.71
(1,579)	1:A:125:VAL:HG13	1:B:205:PRO:HB2	1	0.71
(1,514)	1:A:125:VAL:HB	1:B:205:PRO:HB2	9	0.71
(1,513)	1:A:5:PRO:HB2	1:B:325:VAL:HB	9	0.71
(1,462)	1:B:303:ASN:HA	1:B:305:ASP:HB2	15	0.71

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,326)	1:A:5:PRO:HB3	1:A:6:MET:HA	11	0.71
(1,297)	1:A:19:SER:HA	1:A:20:ASP:HB3	20	0.71
(1,154)	1:B:288:GLU:HB2	1:B:289:ASN:HA	14	0.71
(1,633)	1:A:5:PRO:HB2	1:B:325:VAL:HG21	2	0.7
(1,633)	1:A:5:PRO:HB2	1:B:325:VAL:HG22	2	0.7
(1,633)	1:A:5:PRO:HB2	1:B:325:VAL:HG23	2	0.7
(1,62)	1:B:307:LEU:HB2	1:B:308:PHE:HA	5	0.7
(1,580)	1:A:5:PRO:HB2	1:B:325:VAL:HG11	17	0.7
(1,580)	1:A:5:PRO:HB2	1:B:325:VAL:HG12	17	0.7
(1,580)	1:A:5:PRO:HB2	1:B:325:VAL:HG13	17	0.7
(1,514)	1:A:125:VAL:HB	1:B:205:PRO:HB2	12	0.7
(1,513)	1:A:5:PRO:HB2	1:B:325:VAL:HB	10	0.7
(1,326)	1:A:5:PRO:HB3	1:A:6:MET:HA	14	0.7
(1,166)	1:B:244:LEU:HD11	1:B:286:SER:HA	16	0.7
(1,166)	1:B:244:LEU:HD12	1:B:286:SER:HA	16	0.7
(1,166)	1:B:244:LEU:HD13	1:B:286:SER:HA	16	0.7
(1,154)	1:B:288:GLU:HB2	1:B:289:ASN:HA	20	0.7
(1,153)	1:A:88:GLU:HB2	1:A:89:ASN:HA	14	0.7
(1,1108)	1:A:75:GLU:H	1:B:244:LEU:HD11	8	0.7
(1,1108)	1:A:75:GLU:H	1:B:244:LEU:HD12	8	0.7
(1,1108)	1:A:75:GLU:H	1:B:244:LEU:HD13	8	0.7
(1,328)	1:B:205:PRO:HB3	1:B:206:MET:HA	11	0.69
(1,328)	1:B:205:PRO:HB3	1:B:206:MET:HA	14	0.69
(1,298)	1:B:219:SER:HA	1:B:220:ASP:HB3	20	0.69
(1,159)	1:A:87:ALA:HA	1:A:90:LEU:HD21	2	0.69
(1,159)	1:A:87:ALA:HA	1:A:90:LEU:HD22	2	0.69
(1,159)	1:A:87:ALA:HA	1:A:90:LEU:HD23	2	0.69
(1,159)	1:A:87:ALA:HA	1:A:90:LEU:HD21	15	0.69
(1,159)	1:A:87:ALA:HA	1:A:90:LEU:HD22	15	0.69
(1,159)	1:A:87:ALA:HA	1:A:90:LEU:HD23	15	0.69
(1,153)	1:A:88:GLU:HB2	1:A:89:ASN:HA	20	0.69
(1,1312)	1:B:232:LEU:HD11	1:B:234:ARG:H	5	0.69
(1,1312)	1:B:232:LEU:HD12	1:B:234:ARG:H	5	0.69
(1,1312)	1:B:232:LEU:HD13	1:B:234:ARG:H	5	0.69
(1,1311)	1:A:32:LEU:HD11	1:A:34:ARG:H	5	0.69
(1,1311)	1:A:32:LEU:HD12	1:A:34:ARG:H	5	0.69
(1,1311)	1:A:32:LEU:HD13	1:A:34:ARG:H	5	0.69
(1,1250)	1:B:270:VAL:HG11	1:B:272:MET:H	17	0.69
(1,1250)	1:B:270:VAL:HG12	1:B:272:MET:H	17	0.69
(1,1250)	1:B:270:VAL:HG13	1:B:272:MET:H	17	0.69
(1,800)	1:B:312:ASN:H	1:B:315:LEU:HD21	2	0.68
(1,800)	1:B:312:ASN:H	1:B:315:LEU:HD22	2	0.68

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,800)	1:B:312:ASN:H	1:B:315:LEU:HD23	2	0.68
(1,799)	1:A:112:ASN:H	1:A:115:LEU:HD21	2	0.68
(1,799)	1:A:112:ASN:H	1:A:115:LEU:HD22	2	0.68
(1,799)	1:A:112:ASN:H	1:A:115:LEU:HD23	2	0.68
(1,657)	1:A:93:LEU:HD11	1:A:94:LYS:HG3	15	0.68
(1,657)	1:A:93:LEU:HD12	1:A:94:LYS:HG3	15	0.68
(1,657)	1:A:93:LEU:HD13	1:A:94:LYS:HG3	15	0.68
(1,62)	1:B:307:LEU:HB2	1:B:308:PHE:HA	13	0.68
(1,457)	1:A:102:ARG:HG3	1:A:105:ASP:HB2	17	0.68
(1,328)	1:B:205:PRO:HB3	1:B:206:MET:HA	18	0.68
(1,298)	1:B:219:SER:HA	1:B:220:ASP:HB3	15	0.68
(1,153)	1:A:88:GLU:HB2	1:A:89:ASN:HA	19	0.68
(1,1282)	1:B:293:LEU:HD11	1:B:296:GLU:H	15	0.68
(1,1282)	1:B:293:LEU:HD12	1:B:296:GLU:H	15	0.68
(1,1282)	1:B:293:LEU:HD13	1:B:296:GLU:H	15	0.68
(1,633)	1:A:5:PRO:HB2	1:B:325:VAL:HG21	10	0.67
(1,633)	1:A:5:PRO:HB2	1:B:325:VAL:HG22	10	0.67
(1,633)	1:A:5:PRO:HB2	1:B:325:VAL:HG23	10	0.67
(1,609)	1:A:49:GLY:HA3	1:A:50:GLN:HB2	12	0.67
(1,326)	1:A:5:PRO:HB3	1:A:6:MET:HA	1	0.67
(1,298)	1:B:219:SER:HA	1:B:220:ASP:HB3	11	0.67
(1,298)	1:B:219:SER:HA	1:B:220:ASP:HB3	18	0.67
(1,297)	1:A:19:SER:HA	1:A:20:ASP:HB3	2	0.67
(1,297)	1:A:19:SER:HA	1:A:20:ASP:HB3	18	0.67
(1,164)	1:A:44:LEU:HD11	1:A:86:SER:HA	16	0.67
(1,164)	1:A:44:LEU:HD12	1:A:86:SER:HA	16	0.67
(1,164)	1:A:44:LEU:HD13	1:A:86:SER:HA	16	0.67
(1,154)	1:B:288:GLU:HB2	1:B:289:ASN:HA	19	0.67
(1,667)	1:A:88:GLU:HB2	1:A:89:ASN:HB2	20	0.66
(1,667)	1:A:88:GLU:HB2	1:A:89:ASN:HB3	20	0.66
(1,62)	1:B:307:LEU:HB2	1:B:308:PHE:HA	3	0.66
(1,62)	1:B:307:LEU:HB2	1:B:308:PHE:HA	10	0.66
(1,61)	1:A:107:LEU:HB2	1:A:108:PHE:HA	3	0.66
(1,326)	1:A:5:PRO:HB3	1:A:6:MET:HA	18	0.66
(1,298)	1:B:219:SER:HA	1:B:220:ASP:HB3	2	0.66
(1,160)	1:B:287:ALA:HA	1:B:290:LEU:HD21	2	0.66
(1,160)	1:B:287:ALA:HA	1:B:290:LEU:HD22	2	0.66
(1,160)	1:B:287:ALA:HA	1:B:290:LEU:HD23	2	0.66
(1,668)	1:B:288:GLU:HB2	1:B:289:ASN:HB2	20	0.65
(1,668)	1:B:288:GLU:HB2	1:B:289:ASN:HB3	20	0.65
(1,657)	1:A:93:LEU:HD11	1:A:94:LYS:HG3	6	0.65
(1,657)	1:A:93:LEU:HD12	1:A:94:LYS:HG3	6	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,657)	1:A:93:LEU:HD13	1:A:94:LYS:HG3	6	0.65
(1,61)	1:A:107:LEU:HB2	1:A:108:PHE:HA	13	0.65
(1,553)	1:A:24:LEU:HB3	1:A:26:THR:HA	12	0.65
(1,328)	1:B:205:PRO:HB3	1:B:206:MET:HA	1	0.65
(1,328)	1:B:205:PRO:HB3	1:B:206:MET:HA	3	0.65
(1,326)	1:A:5:PRO:HB3	1:A:6:MET:HA	3	0.65
(1,326)	1:A:5:PRO:HB3	1:A:6:MET:HA	15	0.65
(1,316)	1:B:232:LEU:HA	1:B:250:GLN:HB2	13	0.65
(1,298)	1:B:219:SER:HA	1:B:220:ASP:HB3	17	0.65
(1,1066)	1:B:282:VAL:H	1:B:283:ILE:HG12	19	0.65
(1,1065)	1:A:82:VAL:H	1:A:83:ILE:HG12	1	0.65
(1,717)	1:A:102:ARG:HG2	1:A:125:VAL:H	8	0.64
(1,658)	1:B:293:LEU:HD11	1:B:294:LYS:HG3	15	0.64
(1,658)	1:B:293:LEU:HD12	1:B:294:LYS:HG3	15	0.64
(1,658)	1:B:293:LEU:HD13	1:B:294:LYS:HG3	15	0.64
(1,633)	1:A:5:PRO:HB2	1:B:325:VAL:HG21	16	0.64
(1,633)	1:A:5:PRO:HB2	1:B:325:VAL:HG22	16	0.64
(1,633)	1:A:5:PRO:HB2	1:B:325:VAL:HG23	16	0.64
(1,61)	1:A:107:LEU:HB2	1:A:108:PHE:HA	10	0.64
(1,584)	1:A:75:GLU:HB3	1:B:244:LEU:HD11	8	0.64
(1,584)	1:A:75:GLU:HB3	1:B:244:LEU:HD12	8	0.64
(1,584)	1:A:75:GLU:HB3	1:B:244:LEU:HD13	8	0.64
(1,554)	1:B:224:LEU:HB3	1:B:226:THR:HA	5	0.64
(1,554)	1:B:224:LEU:HB3	1:B:226:THR:HA	19	0.64
(1,393)	1:A:124:ILE:HD11	1:A:125:VAL:HG21	20	0.64
(1,393)	1:A:124:ILE:HD11	1:A:125:VAL:HG22	20	0.64
(1,393)	1:A:124:ILE:HD11	1:A:125:VAL:HG23	20	0.64
(1,393)	1:A:124:ILE:HD12	1:A:125:VAL:HG21	20	0.64
(1,393)	1:A:124:ILE:HD12	1:A:125:VAL:HG22	20	0.64
(1,393)	1:A:124:ILE:HD12	1:A:125:VAL:HG23	20	0.64
(1,393)	1:A:124:ILE:HD13	1:A:125:VAL:HG21	20	0.64
(1,393)	1:A:124:ILE:HD13	1:A:125:VAL:HG22	20	0.64
(1,393)	1:A:124:ILE:HD13	1:A:125:VAL:HG23	20	0.64
(1,328)	1:B:205:PRO:HB3	1:B:206:MET:HA	15	0.64
(1,64)	1:B:307:LEU:HD11	1:B:308:PHE:HA	5	0.63
(1,64)	1:B:307:LEU:HD12	1:B:308:PHE:HA	5	0.63
(1,64)	1:B:307:LEU:HD13	1:B:308:PHE:HA	5	0.63
(1,297)	1:A:19:SER:HA	1:A:20:ASP:HB3	4	0.63
(1,297)	1:A:19:SER:HA	1:A:20:ASP:HB3	9	0.63
(1,1066)	1:B:282:VAL:H	1:B:283:ILE:HG12	13	0.63
(1,635)	1:A:125:VAL:HG21	1:B:205:PRO:HB2	12	0.62
(1,635)	1:A:125:VAL:HG22	1:B:205:PRO:HB2	12	0.62

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,635)	1:A:125:VAL:HG23	1:B:205:PRO:HB2	12	0.62
(1,635)	1:A:125:VAL:HG21	1:B:205:PRO:HB2	16	0.62
(1,635)	1:A:125:VAL:HG22	1:B:205:PRO:HB2	16	0.62
(1,635)	1:A:125:VAL:HG23	1:B:205:PRO:HB2	16	0.62
(1,514)	1:A:125:VAL:HB	1:B:205:PRO:HB2	18	0.62
(1,399)	1:A:102:ARG:HG2	1:A:124:ILE:HD11	20	0.62
(1,399)	1:A:102:ARG:HG2	1:A:124:ILE:HD12	20	0.62
(1,399)	1:A:102:ARG:HG2	1:A:124:ILE:HD13	20	0.62
(1,326)	1:A:5:PRO:HB3	1:A:6:MET:HA	2	0.62
(1,298)	1:B:219:SER:HA	1:B:220:ASP:HB3	4	0.62
(1,298)	1:B:219:SER:HA	1:B:220:ASP:HB3	13	0.62
(1,297)	1:A:19:SER:HA	1:A:20:ASP:HB3	11	0.62
(1,297)	1:A:19:SER:HA	1:A:20:ASP:HB3	17	0.62
(1,224)	1:B:315:LEU:HD21	1:B:316:GLY:HA2	16	0.62
(1,224)	1:B:315:LEU:HD22	1:B:316:GLY:HA2	16	0.62
(1,224)	1:B:315:LEU:HD23	1:B:316:GLY:HA2	16	0.62
(1,1311)	1:A:32:LEU:HD11	1:A:34:ARG:H	18	0.62
(1,1311)	1:A:32:LEU:HD12	1:A:34:ARG:H	18	0.62
(1,1311)	1:A:32:LEU:HD13	1:A:34:ARG:H	18	0.62
(1,1066)	1:B:282:VAL:H	1:B:283:ILE:HG12	1	0.62
(1,635)	1:A:125:VAL:HG21	1:B:205:PRO:HB2	9	0.61
(1,635)	1:A:125:VAL:HG22	1:B:205:PRO:HB2	9	0.61
(1,635)	1:A:125:VAL:HG23	1:B:205:PRO:HB2	9	0.61
(1,633)	1:A:5:PRO:HB2	1:B:325:VAL:HG21	9	0.61
(1,633)	1:A:5:PRO:HB2	1:B:325:VAL:HG22	9	0.61
(1,633)	1:A:5:PRO:HB2	1:B:325:VAL:HG23	9	0.61
(1,62)	1:B:307:LEU:HB2	1:B:308:PHE:HA	12	0.61
(1,328)	1:B:205:PRO:HB3	1:B:206:MET:HA	16	0.61
(1,315)	1:A:32:LEU:HA	1:A:50:GLN:HB2	15	0.61
(1,297)	1:A:19:SER:HA	1:A:20:ASP:HB3	13	0.61
(1,1151)	1:A:33:LEU:H	1:A:49:GLY:HA3	6	0.61
(1,1066)	1:B:282:VAL:H	1:B:283:ILE:HG12	6	0.61
(1,1066)	1:B:282:VAL:H	1:B:283:ILE:HG12	11	0.61
(1,1066)	1:B:282:VAL:H	1:B:283:ILE:HG12	12	0.61
(1,630)	1:B:252:VAL:HG21	1:B:279:ILE:HA	6	0.6
(1,630)	1:B:252:VAL:HG22	1:B:279:ILE:HA	6	0.6
(1,630)	1:B:252:VAL:HG23	1:B:279:ILE:HA	6	0.6
(1,61)	1:A:107:LEU:HB2	1:A:108:PHE:HA	12	0.6
(1,588)	1:B:222:THR:H	1:B:223:ARG:HD3	17	0.6
(1,298)	1:B:219:SER:HA	1:B:220:ASP:HB3	6	0.6
(1,297)	1:A:19:SER:HA	1:A:20:ASP:HB3	6	0.6
(1,224)	1:B:315:LEU:HD21	1:B:316:GLY:HA2	1	0.6

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,224)	1:B:315:LEU:HD22	1:B:316:GLY:HA2	1	0.6
(1,224)	1:B:315:LEU:HD23	1:B:316:GLY:HA2	1	0.6
(1,223)	1:A:115:LEU:HD21	1:A:116:GLY:HA2	1	0.6
(1,223)	1:A:115:LEU:HD22	1:A:116:GLY:HA2	1	0.6
(1,223)	1:A:115:LEU:HD23	1:A:116:GLY:HA2	1	0.6
(1,223)	1:A:115:LEU:HD21	1:A:116:GLY:HA2	8	0.6
(1,223)	1:A:115:LEU:HD22	1:A:116:GLY:HA2	8	0.6
(1,223)	1:A:115:LEU:HD23	1:A:116:GLY:HA2	8	0.6
(1,1065)	1:A:82:VAL:H	1:A:83:ILE:HG12	20	0.6
(1,635)	1:A:125:VAL:HG21	1:B:205:PRO:HB2	5	0.59
(1,635)	1:A:125:VAL:HG22	1:B:205:PRO:HB2	5	0.59
(1,635)	1:A:125:VAL:HG23	1:B:205:PRO:HB2	5	0.59
(1,63)	1:A:107:LEU:HD11	1:A:108:PHE:HA	5	0.59
(1,63)	1:A:107:LEU:HD12	1:A:108:PHE:HA	5	0.59
(1,63)	1:A:107:LEU:HD13	1:A:108:PHE:HA	5	0.59
(1,61)	1:A:107:LEU:HB2	1:A:108:PHE:HA	5	0.59
(1,61)	1:A:107:LEU:HB2	1:A:108:PHE:HA	9	0.59
(1,597)	1:B:249:GLY:H	1:B:250:GLN:HB2	2	0.59
(1,513)	1:A:5:PRO:HB2	1:B:325:VAL:HB	16	0.59
(1,513)	1:A:5:PRO:HB2	1:B:325:VAL:HB	18	0.59
(1,399)	1:A:102:ARG:HG2	1:A:124:ILE:HD11	16	0.59
(1,399)	1:A:102:ARG:HG2	1:A:124:ILE:HD12	16	0.59
(1,399)	1:A:102:ARG:HG2	1:A:124:ILE:HD13	16	0.59
(1,328)	1:B:205:PRO:HB3	1:B:206:MET:HA	2	0.59
(1,326)	1:A:5:PRO:HB3	1:A:6:MET:HA	16	0.59
(1,298)	1:B:219:SER:HA	1:B:220:ASP:HB3	5	0.59
(1,298)	1:B:219:SER:HA	1:B:220:ASP:HB3	9	0.59
(1,297)	1:A:19:SER:HA	1:A:20:ASP:HB3	5	0.59
(1,224)	1:B:315:LEU:HD21	1:B:316:GLY:HA2	8	0.59
(1,224)	1:B:315:LEU:HD22	1:B:316:GLY:HA2	8	0.59
(1,224)	1:B:315:LEU:HD23	1:B:316:GLY:HA2	8	0.59
(1,1260)	1:B:314:GLY:H	1:B:315:LEU:HD21	13	0.59
(1,1260)	1:B:314:GLY:H	1:B:315:LEU:HD22	13	0.59
(1,1260)	1:B:314:GLY:H	1:B:315:LEU:HD23	13	0.59
(1,1260)	1:B:314:GLY:H	1:B:315:LEU:HD21	18	0.59
(1,1260)	1:B:314:GLY:H	1:B:315:LEU:HD22	18	0.59
(1,1260)	1:B:314:GLY:H	1:B:315:LEU:HD23	18	0.59
(1,1259)	1:A:114:GLY:H	1:A:115:LEU:HD21	18	0.59
(1,1259)	1:A:114:GLY:H	1:A:115:LEU:HD22	18	0.59
(1,1259)	1:A:114:GLY:H	1:A:115:LEU:HD23	18	0.59
(1,101)	1:A:93:LEU:HD11	1:A:97:TRP:HA	3	0.59
(1,101)	1:A:93:LEU:HD12	1:A:97:TRP:HA	3	0.59

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,101)	1:A:93:LEU:HD13	1:A:97:TRP:HA	3	0.59
(1,635)	1:A:125:VAL:HG21	1:B:205:PRO:HB2	18	0.58
(1,635)	1:A:125:VAL:HG22	1:B:205:PRO:HB2	18	0.58
(1,635)	1:A:125:VAL:HG23	1:B:205:PRO:HB2	18	0.58
(1,328)	1:B:205:PRO:HB3	1:B:206:MET:HA	12	0.58
(1,260)	1:B:228:PHE:HA	1:B:252:VAL:HB	14	0.58
(1,163)	1:A:47:VAL:HG21	1:A:86:SER:HA	15	0.58
(1,163)	1:A:47:VAL:HG22	1:A:86:SER:HA	15	0.58
(1,163)	1:A:47:VAL:HG23	1:A:86:SER:HA	15	0.58
(1,1268)	1:B:217:VAL:HG11	1:B:219:SER:H	11	0.58
(1,1268)	1:B:217:VAL:HG12	1:B:219:SER:H	11	0.58
(1,1268)	1:B:217:VAL:HG13	1:B:219:SER:H	11	0.58
(1,1259)	1:A:114:GLY:H	1:A:115:LEU:HD21	14	0.58
(1,1259)	1:A:114:GLY:H	1:A:115:LEU:HD22	14	0.58
(1,1259)	1:A:114:GLY:H	1:A:115:LEU:HD23	14	0.58
(1,1066)	1:B:282:VAL:H	1:B:283:ILE:HG12	20	0.58
(1,648)	1:B:302:ARG:HG2	1:B:325:VAL:HA	17	0.57
(1,633)	1:A:5:PRO:HB2	1:B:325:VAL:HG21	1	0.57
(1,633)	1:A:5:PRO:HB2	1:B:325:VAL:HG22	1	0.57
(1,633)	1:A:5:PRO:HB2	1:B:325:VAL:HG23	1	0.57
(1,553)	1:A:24:LEU:HB3	1:A:26:THR:HA	18	0.57
(1,549)	1:B:220:ASP:HB2	1:B:221:PRO:HB2	17	0.57
(1,298)	1:B:219:SER:HA	1:B:220:ASP:HB3	3	0.57
(1,297)	1:A:19:SER:HA	1:A:20:ASP:HB3	1	0.57
(1,297)	1:A:19:SER:HA	1:A:20:ASP:HB3	3	0.57
(1,223)	1:A:115:LEU:HD21	1:A:116:GLY:HA2	16	0.57
(1,223)	1:A:115:LEU:HD22	1:A:116:GLY:HA2	16	0.57
(1,223)	1:A:115:LEU:HD23	1:A:116:GLY:HA2	16	0.57
(1,1267)	1:A:17:VAL:HG11	1:A:19:SER:H	18	0.57
(1,1267)	1:A:17:VAL:HG12	1:A:19:SER:H	18	0.57
(1,1267)	1:A:17:VAL:HG13	1:A:19:SER:H	18	0.57
(1,1260)	1:B:314:GLY:H	1:B:315:LEU:HD21	14	0.57
(1,1260)	1:B:314:GLY:H	1:B:315:LEU:HD22	14	0.57
(1,1260)	1:B:314:GLY:H	1:B:315:LEU:HD23	14	0.57
(1,1107)	1:A:44:LEU:HD11	1:B:275:GLU:H	8	0.57
(1,1107)	1:A:44:LEU:HD12	1:B:275:GLU:H	8	0.57
(1,1107)	1:A:44:LEU:HD13	1:B:275:GLU:H	8	0.57
(1,1065)	1:A:82:VAL:H	1:A:83:ILE:HG12	11	0.57
(1,1065)	1:A:82:VAL:H	1:A:83:ILE:HG12	13	0.57
(1,582)	1:A:44:LEU:HD11	1:B:275:GLU:HB3	8	0.56
(1,582)	1:A:44:LEU:HD12	1:B:275:GLU:HB3	8	0.56
(1,582)	1:A:44:LEU:HD13	1:B:275:GLU:HB3	8	0.56

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,326)	1:A:5:PRO:HB3	1:A:6:MET:HA	12	0.56
(1,304)	1:A:31:SER:HA	1:A:50:GLN:H	19	0.56
(1,1223)	1:A:17:VAL:HG11	1:A:29:SER:H	8	0.56
(1,1223)	1:A:17:VAL:HG12	1:A:29:SER:H	8	0.56
(1,1223)	1:A:17:VAL:HG13	1:A:29:SER:H	8	0.56
(1,1152)	1:B:233:LEU:H	1:B:249:GLY:HA3	6	0.56
(1,1087)	1:B:278:SER:H	1:B:279:ILE:HG12	19	0.56
(1,1065)	1:A:82:VAL:H	1:A:83:ILE:HG12	8	0.56
(1,633)	1:A:5:PRO:HB2	1:B:325:VAL:HG21	18	0.55
(1,633)	1:A:5:PRO:HB2	1:B:325:VAL:HG22	18	0.55
(1,633)	1:A:5:PRO:HB2	1:B:325:VAL:HG23	18	0.55
(1,616)	1:A:102:ARG:HB2	1:A:103:ASN:HB2	6	0.55
(1,616)	1:A:102:ARG:HB3	1:A:103:ASN:HB2	6	0.55
(1,589)	1:A:23:ARG:HA	1:A:23:ARG:HD3	17	0.55
(1,298)	1:B:219:SER:HA	1:B:220:ASP:HB3	19	0.55
(1,260)	1:B:228:PHE:HA	1:B:252:VAL:HB	7	0.55
(1,224)	1:B:315:LEU:HD21	1:B:316:GLY:HA2	19	0.55
(1,224)	1:B:315:LEU:HD22	1:B:316:GLY:HA2	19	0.55
(1,224)	1:B:315:LEU:HD23	1:B:316:GLY:HA2	19	0.55
(1,223)	1:A:115:LEU:HD21	1:A:116:GLY:HA2	19	0.55
(1,223)	1:A:115:LEU:HD22	1:A:116:GLY:HA2	19	0.55
(1,223)	1:A:115:LEU:HD23	1:A:116:GLY:HA2	19	0.55
(1,1260)	1:B:314:GLY:H	1:B:315:LEU:HD21	15	0.55
(1,1260)	1:B:314:GLY:H	1:B:315:LEU:HD22	15	0.55
(1,1260)	1:B:314:GLY:H	1:B:315:LEU:HD23	15	0.55
(1,1259)	1:A:114:GLY:H	1:A:115:LEU:HD21	12	0.55
(1,1259)	1:A:114:GLY:H	1:A:115:LEU:HD22	12	0.55
(1,1259)	1:A:114:GLY:H	1:A:115:LEU:HD23	12	0.55
(1,1066)	1:B:282:VAL:H	1:B:283:ILE:HG12	16	0.55
(1,1065)	1:A:82:VAL:H	1:A:83:ILE:HG12	10	0.55
(1,1065)	1:A:82:VAL:H	1:A:83:ILE:HG12	12	0.55
(1,98)	1:B:270:VAL:HG11	1:B:271:ILE:HA	10	0.54
(1,98)	1:B:270:VAL:HG12	1:B:271:ILE:HA	10	0.54
(1,98)	1:B:270:VAL:HG13	1:B:271:ILE:HA	10	0.54
(1,635)	1:A:125:VAL:HG21	1:B:205:PRO:HB2	14	0.54
(1,635)	1:A:125:VAL:HG22	1:B:205:PRO:HB2	14	0.54
(1,635)	1:A:125:VAL:HG23	1:B:205:PRO:HB2	14	0.54
(1,61)	1:A:107:LEU:HB2	1:A:108:PHE:HA	11	0.54
(1,550)	1:B:269:CYS:HB3	1:B:270:VAL:HB	16	0.54
(1,514)	1:A:125:VAL:HB	1:B:205:PRO:HB2	16	0.54
(1,297)	1:A:19:SER:HA	1:A:20:ASP:HB3	15	0.54
(1,259)	1:B:217:VAL:HB	1:B:228:PHE:HA	3	0.54

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,165)	1:B:247:VAL:HG21	1:B:286:SER:HA	4	0.54
(1,165)	1:B:247:VAL:HG22	1:B:286:SER:HA	4	0.54
(1,165)	1:B:247:VAL:HG23	1:B:286:SER:HA	4	0.54
(1,160)	1:B:287:ALA:HA	1:B:290:LEU:HD21	19	0.54
(1,160)	1:B:287:ALA:HA	1:B:290:LEU:HD22	19	0.54
(1,160)	1:B:287:ALA:HA	1:B:290:LEU:HD23	19	0.54
(1,1259)	1:A:114:GLY:H	1:A:115:LEU:HD21	15	0.54
(1,1259)	1:A:114:GLY:H	1:A:115:LEU:HD22	15	0.54
(1,1259)	1:A:114:GLY:H	1:A:115:LEU:HD23	15	0.54
(1,1151)	1:A:33:LEU:H	1:A:49:GLY:HA3	13	0.54
(1,1085)	1:A:78:SER:H	1:A:79:ILE:HG12	19	0.54
(1,1065)	1:A:82:VAL:H	1:A:83:ILE:HG12	16	0.54
(1,96)	1:A:70:VAL:HG11	1:A:71:ILE:HA	20	0.53
(1,96)	1:A:70:VAL:HG12	1:A:71:ILE:HA	20	0.53
(1,96)	1:A:70:VAL:HG13	1:A:71:ILE:HA	20	0.53
(1,616)	1:A:102:ARG:HB2	1:A:103:ASN:HB2	8	0.53
(1,616)	1:A:102:ARG:HB3	1:A:103:ASN:HB2	8	0.53
(1,257)	1:A:17:VAL:HB	1:A:28:PHE:HA	13	0.53
(1,224)	1:B:315:LEU:HD21	1:B:316:GLY:HA2	9	0.53
(1,224)	1:B:315:LEU:HD22	1:B:316:GLY:HA2	9	0.53
(1,224)	1:B:315:LEU:HD23	1:B:316:GLY:HA2	9	0.53
(1,223)	1:A:115:LEU:HD21	1:A:116:GLY:HA2	7	0.53
(1,223)	1:A:115:LEU:HD22	1:A:116:GLY:HA2	7	0.53
(1,223)	1:A:115:LEU:HD23	1:A:116:GLY:HA2	7	0.53
(1,1065)	1:A:82:VAL:H	1:A:83:ILE:HG12	2	0.53
(1,782)	1:B:315:LEU:H	1:B:316:GLY:HA3	1	0.52
(1,781)	1:A:115:LEU:H	1:A:116:GLY:HA3	1	0.52
(1,627)	1:A:52:VAL:HG21	1:A:54:VAL:HA	19	0.52
(1,627)	1:A:52:VAL:HG22	1:A:54:VAL:HA	19	0.52
(1,627)	1:A:52:VAL:HG23	1:A:54:VAL:HA	19	0.52
(1,62)	1:B:307:LEU:HB2	1:B:308:PHE:HA	11	0.52
(1,507)	1:A:54:VAL:HB	1:A:78:SER:HA	16	0.52
(1,497)	1:A:20:ASP:HB2	1:A:23:ARG:HD3	3	0.52
(1,316)	1:B:232:LEU:HA	1:B:250:GLN:HB2	11	0.52
(1,258)	1:A:28:PHE:HA	1:A:52:VAL:HB	19	0.52
(1,224)	1:B:315:LEU:HD21	1:B:316:GLY:HA2	7	0.52
(1,224)	1:B:315:LEU:HD22	1:B:316:GLY:HA2	7	0.52
(1,224)	1:B:315:LEU:HD23	1:B:316:GLY:HA2	7	0.52
(1,224)	1:B:315:LEU:HD21	1:B:316:GLY:HA2	17	0.52
(1,224)	1:B:315:LEU:HD22	1:B:316:GLY:HA2	17	0.52
(1,224)	1:B:315:LEU:HD23	1:B:316:GLY:HA2	17	0.52
(1,223)	1:A:115:LEU:HD21	1:A:116:GLY:HA2	9	0.52

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,223)	1:A:115:LEU:HD22	1:A:116:GLY:HA2	9	0.52
(1,223)	1:A:115:LEU:HD23	1:A:116:GLY:HA2	9	0.52
(1,1065)	1:A:82:VAL:H	1:A:83:ILE:HG12	14	0.52
(1,782)	1:B:315:LEU:H	1:B:316:GLY:HA3	8	0.51
(1,781)	1:A:115:LEU:H	1:A:116:GLY:HA3	8	0.51
(1,741)	1:A:124:ILE:H	1:A:124:ILE:HG12	18	0.51
(1,658)	1:B:293:LEU:HD11	1:B:294:LYS:HG3	5	0.51
(1,658)	1:B:293:LEU:HD12	1:B:294:LYS:HG3	5	0.51
(1,658)	1:B:293:LEU:HD13	1:B:294:LYS:HG3	5	0.51
(1,634)	1:A:69:CYS:HB2	1:A:70:VAL:HG11	15	0.51
(1,634)	1:A:69:CYS:HB2	1:A:70:VAL:HG12	15	0.51
(1,634)	1:A:69:CYS:HB2	1:A:70:VAL:HG13	15	0.51
(1,62)	1:B:307:LEU:HB2	1:B:308:PHE:HA	9	0.51
(1,482)	1:B:302:ARG:H	1:B:302:ARG:HD3	14	0.51
(1,462)	1:B:303:ASN:HA	1:B:305:ASP:HB2	3	0.51
(1,298)	1:B:219:SER:HA	1:B:220:ASP:HB3	12	0.51
(1,258)	1:A:28:PHE:HA	1:A:52:VAL:HB	8	0.51
(1,223)	1:A:115:LEU:HD21	1:A:116:GLY:HA2	17	0.51
(1,223)	1:A:115:LEU:HD22	1:A:116:GLY:HA2	17	0.51
(1,223)	1:A:115:LEU:HD23	1:A:116:GLY:HA2	17	0.51
(1,159)	1:A:87:ALA:HA	1:A:90:LEU:HD21	19	0.51
(1,159)	1:A:87:ALA:HA	1:A:90:LEU:HD22	19	0.51
(1,159)	1:A:87:ALA:HA	1:A:90:LEU:HD23	19	0.51
(1,1065)	1:A:82:VAL:H	1:A:83:ILE:HG12	9	0.51
(1,101)	1:A:93:LEU:HD11	1:A:97:TRP:HA	2	0.51
(1,101)	1:A:93:LEU:HD12	1:A:97:TRP:HA	2	0.51
(1,101)	1:A:93:LEU:HD13	1:A:97:TRP:HA	2	0.51
(1,782)	1:B:315:LEU:H	1:B:316:GLY:HA3	19	0.5
(1,742)	1:B:324:ILE:H	1:B:324:ILE:HG12	18	0.5
(1,741)	1:A:124:ILE:H	1:A:124:ILE:HG12	11	0.5
(1,647)	1:A:102:ARG:HG2	1:A:125:VAL:HA	17	0.5
(1,548)	1:A:69:CYS:HB3	1:A:70:VAL:HB	10	0.5
(1,400)	1:B:302:ARG:HG2	1:B:324:ILE:HD11	17	0.5
(1,400)	1:B:302:ARG:HG2	1:B:324:ILE:HD12	17	0.5
(1,400)	1:B:302:ARG:HG2	1:B:324:ILE:HD13	17	0.5
(1,376)	1:B:217:VAL:HB	1:B:227:THR:HB	17	0.5
(1,1225)	1:B:217:VAL:HG11	1:B:229:SER:H	1	0.5
(1,1225)	1:B:217:VAL:HG12	1:B:229:SER:H	1	0.5
(1,1225)	1:B:217:VAL:HG13	1:B:229:SER:H	1	0.5
(1,1107)	1:A:44:LEU:HD11	1:B:275:GLU:H	3	0.5
(1,1107)	1:A:44:LEU:HD12	1:B:275:GLU:H	3	0.5
(1,1107)	1:A:44:LEU:HD13	1:B:275:GLU:H	3	0.5

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1066)	1:B:282:VAL:H	1:B:283:ILE:HG12	10	0.5
(1,781)	1:A:115:LEU:H	1:A:116:GLY:HA3	19	0.49
(1,741)	1:A:124:ILE:H	1:A:124:ILE:HG12	4	0.49
(1,741)	1:A:124:ILE:H	1:A:124:ILE:HG12	9	0.49
(1,657)	1:A:93:LEU:HD11	1:A:94:LYS:HG3	5	0.49
(1,657)	1:A:93:LEU:HD12	1:A:94:LYS:HG3	5	0.49
(1,657)	1:A:93:LEU:HD13	1:A:94:LYS:HG3	5	0.49
(1,585)	1:A:75:GLU:HG3	1:A:76:ASN:H	14	0.49
(1,526)	1:A:16:ILE:HB	1:A:29:SER:HA	5	0.49
(1,497)	1:A:20:ASP:HB2	1:A:23:ARG:HD3	1	0.49
(1,481)	1:A:102:ARG:H	1:A:102:ARG:HD3	14	0.49
(1,257)	1:A:17:VAL:HB	1:A:28:PHE:HA	19	0.49
(1,164)	1:A:44:LEU:HD11	1:A:86:SER:HA	8	0.49
(1,164)	1:A:44:LEU:HD12	1:A:86:SER:HA	8	0.49
(1,164)	1:A:44:LEU:HD13	1:A:86:SER:HA	8	0.49
(1,1225)	1:B:217:VAL:HG11	1:B:229:SER:H	14	0.49
(1,1225)	1:B:217:VAL:HG12	1:B:229:SER:H	14	0.49
(1,1225)	1:B:217:VAL:HG13	1:B:229:SER:H	14	0.49
(1,1066)	1:B:282:VAL:H	1:B:283:ILE:HG12	8	0.49
(1,1066)	1:B:282:VAL:H	1:B:283:ILE:HG12	18	0.49
(1,782)	1:B:315:LEU:H	1:B:316:GLY:HA3	11	0.48
(1,782)	1:B:315:LEU:H	1:B:316:GLY:HA3	16	0.48
(1,640)	1:B:319:ASP:H	1:B:321:THR:HG21	20	0.48
(1,640)	1:B:319:ASP:H	1:B:321:THR:HG22	20	0.48
(1,640)	1:B:319:ASP:H	1:B:321:THR:HG23	20	0.48
(1,597)	1:B:249:GLY:H	1:B:250:GLN:HB2	16	0.48
(1,596)	1:B:303:ASN:H	1:B:304:VAL:HB	5	0.48
(1,547)	1:A:20:ASP:HB2	1:A:21:PRO:HB2	4	0.48
(1,545)	1:A:27:THR:HB	1:A:54:VAL:HB	1	0.48
(1,515)	1:A:125:VAL:HB	1:A:126:SER:HB2	20	0.48
(1,515)	1:A:125:VAL:HB	1:A:126:SER:HB3	20	0.48
(1,514)	1:A:125:VAL:HB	1:B:205:PRO:HB2	14	0.48
(1,498)	1:B:220:ASP:HB2	1:B:223:ARG:HD3	3	0.48
(1,461)	1:A:103:ASN:HA	1:A:105:ASP:HB2	5	0.48
(1,1260)	1:B:314:GLY:H	1:B:315:LEU:HD21	12	0.48
(1,1260)	1:B:314:GLY:H	1:B:315:LEU:HD22	12	0.48
(1,1260)	1:B:314:GLY:H	1:B:315:LEU:HD23	12	0.48
(1,1065)	1:A:82:VAL:H	1:A:83:ILE:HG12	6	0.48
(1,742)	1:B:324:ILE:H	1:B:324:ILE:HG12	9	0.47
(1,534)	1:B:250:GLN:HA	1:B:282:VAL:HB	12	0.47
(1,400)	1:B:302:ARG:HG2	1:B:324:ILE:HD11	3	0.47
(1,400)	1:B:302:ARG:HG2	1:B:324:ILE:HD12	3	0.47

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,400)	1:B:302:ARG:HG2	1:B:324:ILE:HD13	3	0.47
(1,399)	1:A:102:ARG:HG2	1:A:124:ILE:HD11	3	0.47
(1,399)	1:A:102:ARG:HG2	1:A:124:ILE:HD12	3	0.47
(1,399)	1:A:102:ARG:HG2	1:A:124:ILE:HD13	3	0.47
(1,260)	1:B:228:PHE:HA	1:B:252:VAL:HB	19	0.47
(1,224)	1:B:315:LEU:HD21	1:B:316:GLY:HA2	10	0.47
(1,224)	1:B:315:LEU:HD22	1:B:316:GLY:HA2	10	0.47
(1,224)	1:B:315:LEU:HD23	1:B:316:GLY:HA2	10	0.47
(1,166)	1:B:244:LEU:HD11	1:B:286:SER:HA	8	0.47
(1,166)	1:B:244:LEU:HD12	1:B:286:SER:HA	8	0.47
(1,166)	1:B:244:LEU:HD13	1:B:286:SER:HA	8	0.47
(1,1065)	1:A:82:VAL:H	1:A:83:ILE:HG12	4	0.47
(1,1065)	1:A:82:VAL:H	1:A:83:ILE:HG12	15	0.47
(1,636)	1:B:269:CYS:HB2	1:B:270:VAL:HG11	14	0.46
(1,636)	1:B:269:CYS:HB2	1:B:270:VAL:HG12	14	0.46
(1,636)	1:B:269:CYS:HB2	1:B:270:VAL:HG13	14	0.46
(1,583)	1:A:73:PRO:HB3	1:B:244:LEU:HD11	15	0.46
(1,583)	1:A:73:PRO:HB3	1:B:244:LEU:HD12	15	0.46
(1,583)	1:A:73:PRO:HB3	1:B:244:LEU:HD13	15	0.46
(1,549)	1:B:220:ASP:HB2	1:B:221:PRO:HB2	4	0.46
(1,548)	1:A:69:CYS:HB3	1:A:70:VAL:HB	6	0.46
(1,461)	1:A:103:ASN:HA	1:A:105:ASP:HB2	9	0.46
(1,286)	1:B:251:TYR:H	1:B:280:ARG:HA	12	0.46
(1,285)	1:A:51:TYR:H	1:A:80:ARG:HA	19	0.46
(1,1216)	1:B:231:SER:H	1:B:252:VAL:HG11	17	0.46
(1,1216)	1:B:231:SER:H	1:B:252:VAL:HG12	17	0.46
(1,1216)	1:B:231:SER:H	1:B:252:VAL:HG13	17	0.46
(1,102)	1:B:293:LEU:HD11	1:B:297:TRP:HA	18	0.46
(1,102)	1:B:293:LEU:HD12	1:B:297:TRP:HA	18	0.46
(1,102)	1:B:293:LEU:HD13	1:B:297:TRP:HA	18	0.46
(1,782)	1:B:315:LEU:H	1:B:316:GLY:HA3	4	0.45
(1,782)	1:B:315:LEU:H	1:B:316:GLY:HA3	7	0.45
(1,782)	1:B:315:LEU:H	1:B:316:GLY:HA3	17	0.45
(1,781)	1:A:115:LEU:H	1:A:116:GLY:HA3	4	0.45
(1,781)	1:A:115:LEU:H	1:A:116:GLY:HA3	17	0.45
(1,742)	1:B:324:ILE:H	1:B:324:ILE:HG12	10	0.45
(1,742)	1:B:324:ILE:H	1:B:324:ILE:HG12	19	0.45
(1,741)	1:A:124:ILE:H	1:A:124:ILE:HG12	10	0.45
(1,588)	1:B:222:THR:H	1:B:223:ARG:HD3	16	0.45
(1,399)	1:A:102:ARG:HG2	1:A:124:ILE:HD11	17	0.45
(1,399)	1:A:102:ARG:HG2	1:A:124:ILE:HD12	17	0.45
(1,399)	1:A:102:ARG:HG2	1:A:124:ILE:HD13	17	0.45

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,315)	1:A:32:LEU:HA	1:A:50:GLN:HB2	12	0.45
(1,224)	1:B:315:LEU:HD21	1:B:316:GLY:HA2	3	0.45
(1,224)	1:B:315:LEU:HD22	1:B:316:GLY:HA2	3	0.45
(1,224)	1:B:315:LEU:HD23	1:B:316:GLY:HA2	3	0.45
(1,223)	1:A:115:LEU:HD21	1:A:116:GLY:HA2	3	0.45
(1,223)	1:A:115:LEU:HD22	1:A:116:GLY:HA2	3	0.45
(1,223)	1:A:115:LEU:HD23	1:A:116:GLY:HA2	3	0.45
(1,1066)	1:B:282:VAL:H	1:B:283:ILE:HG12	4	0.45
(1,1065)	1:A:82:VAL:H	1:A:83:ILE:HG12	7	0.45
(1,782)	1:B:315:LEU:H	1:B:316:GLY:HA3	2	0.44
(1,782)	1:B:315:LEU:H	1:B:316:GLY:HA3	9	0.44
(1,781)	1:A:115:LEU:H	1:A:116:GLY:HA3	2	0.44
(1,781)	1:A:115:LEU:H	1:A:116:GLY:HA3	16	0.44
(1,741)	1:A:124:ILE:H	1:A:124:ILE:HG12	19	0.44
(1,586)	1:B:275:GLU:HG3	1:B:276:ASN:H	14	0.44
(1,547)	1:A:20:ASP:HB2	1:A:21:PRO:HB2	1	0.44
(1,482)	1:B:302:ARG:H	1:B:302:ARG:HD3	18	0.44
(1,315)	1:A:32:LEU:HA	1:A:50:GLN:HB2	16	0.44
(1,166)	1:B:244:LEU:HD11	1:B:286:SER:HA	17	0.44
(1,166)	1:B:244:LEU:HD12	1:B:286:SER:HA	17	0.44
(1,166)	1:B:244:LEU:HD13	1:B:286:SER:HA	17	0.44
(1,153)	1:A:88:GLU:HB2	1:A:89:ASN:HA	17	0.44
(1,1312)	1:B:232:LEU:HD11	1:B:234:ARG:H	18	0.44
(1,1312)	1:B:232:LEU:HD12	1:B:234:ARG:H	18	0.44
(1,1312)	1:B:232:LEU:HD13	1:B:234:ARG:H	18	0.44
(1,959)	1:A:92:THR:HG21	1:A:95:ALA:H	4	0.43
(1,959)	1:A:92:THR:HG22	1:A:95:ALA:H	4	0.43
(1,959)	1:A:92:THR:HG23	1:A:95:ALA:H	4	0.43
(1,781)	1:A:115:LEU:H	1:A:116:GLY:HA3	9	0.43
(1,641)	1:A:53:SER:H	1:A:54:VAL:HG21	6	0.43
(1,641)	1:A:53:SER:H	1:A:54:VAL:HG22	6	0.43
(1,641)	1:A:53:SER:H	1:A:54:VAL:HG23	6	0.43
(1,634)	1:A:69:CYS:HB2	1:A:70:VAL:HG11	11	0.43
(1,634)	1:A:69:CYS:HB2	1:A:70:VAL:HG12	11	0.43
(1,634)	1:A:69:CYS:HB2	1:A:70:VAL:HG13	11	0.43
(1,517)	1:B:325:VAL:HB	1:B:326:SER:HB2	17	0.43
(1,517)	1:B:325:VAL:HB	1:B:326:SER:HB3	17	0.43
(1,481)	1:A:102:ARG:H	1:A:102:ARG:HD3	18	0.43
(1,394)	1:B:324:ILE:HD11	1:B:325:VAL:HG21	17	0.43
(1,394)	1:B:324:ILE:HD11	1:B:325:VAL:HG22	17	0.43
(1,394)	1:B:324:ILE:HD11	1:B:325:VAL:HG23	17	0.43
(1,394)	1:B:324:ILE:HD12	1:B:325:VAL:HG21	17	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,394)	1:B:324:ILE:HD12	1:B:325:VAL:HG22	17	0.43
(1,394)	1:B:324:ILE:HD12	1:B:325:VAL:HG23	17	0.43
(1,394)	1:B:324:ILE:HD13	1:B:325:VAL:HG21	17	0.43
(1,394)	1:B:324:ILE:HD13	1:B:325:VAL:HG22	17	0.43
(1,394)	1:B:324:ILE:HD13	1:B:325:VAL:HG23	17	0.43
(1,320)	1:B:274:ASN:HB3	1:B:275:GLU:HA	4	0.43
(1,320)	1:B:274:ASN:HB3	1:B:275:GLU:HA	14	0.43
(1,318)	1:A:74:ASN:HB3	1:A:75:GLU:HA	3	0.43
(1,318)	1:A:74:ASN:HB3	1:A:75:GLU:HA	4	0.43
(1,318)	1:A:74:ASN:HB3	1:A:75:GLU:HA	9	0.43
(1,30)	1:B:232:LEU:HD11	1:B:233:LEU:HA	13	0.43
(1,30)	1:B:232:LEU:HD12	1:B:233:LEU:HA	13	0.43
(1,30)	1:B:232:LEU:HD13	1:B:233:LEU:HA	13	0.43
(1,1267)	1:A:17:VAL:HG11	1:A:19:SER:H	12	0.43
(1,1267)	1:A:17:VAL:HG12	1:A:19:SER:H	12	0.43
(1,1267)	1:A:17:VAL:HG13	1:A:19:SER:H	12	0.43
(1,1066)	1:B:282:VAL:H	1:B:283:ILE:HG12	2	0.43
(1,1066)	1:B:282:VAL:H	1:B:283:ILE:HG12	15	0.43
(1,1066)	1:B:282:VAL:H	1:B:283:ILE:HG12	17	0.43
(1,95)	1:A:32:LEU:HD11	1:A:34:ARG:HA	20	0.42
(1,95)	1:A:32:LEU:HD12	1:A:34:ARG:HA	20	0.42
(1,95)	1:A:32:LEU:HD13	1:A:34:ARG:HA	20	0.42
(1,781)	1:A:115:LEU:H	1:A:116:GLY:HA3	7	0.42
(1,781)	1:A:115:LEU:H	1:A:116:GLY:HA3	11	0.42
(1,515)	1:A:125:VAL:HB	1:A:126:SER:HB2	1	0.42
(1,515)	1:A:125:VAL:HB	1:A:126:SER:HB3	1	0.42
(1,320)	1:B:274:ASN:HB3	1:B:275:GLU:HA	9	0.42
(1,318)	1:A:74:ASN:HB3	1:A:75:GLU:HA	13	0.42
(1,164)	1:A:44:LEU:HD11	1:A:86:SER:HA	17	0.42
(1,164)	1:A:44:LEU:HD12	1:A:86:SER:HA	17	0.42
(1,164)	1:A:44:LEU:HD13	1:A:86:SER:HA	17	0.42
(1,1225)	1:B:217:VAL:HG11	1:B:229:SER:H	12	0.42
(1,1225)	1:B:217:VAL:HG12	1:B:229:SER:H	12	0.42
(1,1225)	1:B:217:VAL:HG13	1:B:229:SER:H	12	0.42
(1,782)	1:B:315:LEU:H	1:B:316:GLY:HA3	10	0.41
(1,781)	1:A:115:LEU:H	1:A:116:GLY:HA3	20	0.41
(1,742)	1:B:324:ILE:H	1:B:324:ILE:HG12	16	0.41
(1,628)	1:A:52:VAL:HG21	1:A:79:ILE:HA	1	0.41
(1,628)	1:A:52:VAL:HG22	1:A:79:ILE:HA	1	0.41
(1,628)	1:A:52:VAL:HG23	1:A:79:ILE:HA	1	0.41
(1,462)	1:B:303:ASN:HA	1:B:305:ASP:HB2	10	0.41
(1,459)	1:B:302:ARG:HB2	1:B:305:ASP:HB2	11	0.41

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,459)	1:B:302:ARG:HB3	1:B:305:ASP:HB2	11	0.41
(1,456)	1:A:102:ARG:HB2	1:A:105:ASP:HB2	11	0.41
(1,456)	1:A:102:ARG:HB3	1:A:105:ASP:HB2	11	0.41
(1,318)	1:A:74:ASN:HB3	1:A:75:GLU:HA	14	0.41
(1,1152)	1:B:233:LEU:H	1:B:249:GLY:HA3	13	0.41
(1,1035)	1:A:84:SER:H	1:B:279:ILE:HG12	19	0.41
(1,96)	1:A:70:VAL:HG11	1:A:71:ILE:HA	12	0.4
(1,96)	1:A:70:VAL:HG12	1:A:71:ILE:HA	12	0.4
(1,96)	1:A:70:VAL:HG13	1:A:71:ILE:HA	12	0.4
(1,96)	1:A:70:VAL:HG11	1:A:71:ILE:HA	16	0.4
(1,96)	1:A:70:VAL:HG12	1:A:71:ILE:HA	16	0.4
(1,96)	1:A:70:VAL:HG13	1:A:71:ILE:HA	16	0.4
(1,782)	1:B:315:LEU:H	1:B:316:GLY:HA3	15	0.4
(1,781)	1:A:115:LEU:H	1:A:116:GLY:HA3	10	0.4
(1,781)	1:A:115:LEU:H	1:A:116:GLY:HA3	15	0.4
(1,723)	1:B:303:ASN:HB3	1:B:325:VAL:H	19	0.4
(1,720)	1:A:103:ASN:HB3	1:A:125:VAL:H	16	0.4
(1,720)	1:A:103:ASN:HB3	1:A:125:VAL:H	19	0.4
(1,636)	1:B:269:CYS:HB2	1:B:270:VAL:HG11	1	0.4
(1,636)	1:B:269:CYS:HB2	1:B:270:VAL:HG12	1	0.4
(1,636)	1:B:269:CYS:HB2	1:B:270:VAL:HG13	1	0.4
(1,636)	1:B:269:CYS:HB2	1:B:270:VAL:HG11	18	0.4
(1,636)	1:B:269:CYS:HB2	1:B:270:VAL:HG12	18	0.4
(1,636)	1:B:269:CYS:HB2	1:B:270:VAL:HG13	18	0.4
(1,634)	1:A:69:CYS:HB2	1:A:70:VAL:HG11	13	0.4
(1,634)	1:A:69:CYS:HB2	1:A:70:VAL:HG12	13	0.4
(1,634)	1:A:69:CYS:HB2	1:A:70:VAL:HG13	13	0.4
(1,616)	1:A:102:ARG:HB2	1:A:103:ASN:HB2	1	0.4
(1,616)	1:A:102:ARG:HB3	1:A:103:ASN:HB2	1	0.4
(1,614)	1:B:220:ASP:HA	1:B:223:ARG:HB2	14	0.4
(1,549)	1:B:220:ASP:HB2	1:B:221:PRO:HB2	19	0.4
(1,320)	1:B:274:ASN:HB3	1:B:275:GLU:HA	13	0.4
(1,154)	1:B:288:GLU:HB2	1:B:289:ASN:HA	17	0.4
(1,1311)	1:A:32:LEU:HD11	1:A:34:ARG:H	19	0.4
(1,1311)	1:A:32:LEU:HD12	1:A:34:ARG:H	19	0.4
(1,1311)	1:A:32:LEU:HD13	1:A:34:ARG:H	19	0.4
(1,1268)	1:B:217:VAL:HG11	1:B:219:SER:H	12	0.4
(1,1268)	1:B:217:VAL:HG12	1:B:219:SER:H	12	0.4
(1,1268)	1:B:217:VAL:HG13	1:B:219:SER:H	12	0.4
(1,1210)	1:B:227:THR:H	1:B:254:VAL:HB	11	0.4
(1,1066)	1:B:282:VAL:H	1:B:283:ILE:HG12	9	0.4
(1,782)	1:B:315:LEU:H	1:B:316:GLY:HA3	3	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,782)	1:B:315:LEU:H	1:B:316:GLY:HA3	13	0.39
(1,782)	1:B:315:LEU:H	1:B:316:GLY:HA3	14	0.39
(1,782)	1:B:315:LEU:H	1:B:316:GLY:HA3	18	0.39
(1,781)	1:A:115:LEU:H	1:A:116:GLY:HA3	14	0.39
(1,781)	1:A:115:LEU:H	1:A:116:GLY:HA3	18	0.39
(1,742)	1:B:324:ILE:H	1:B:324:ILE:HG12	14	0.39
(1,641)	1:A:53:SER:H	1:A:54:VAL:HG21	1	0.39
(1,641)	1:A:53:SER:H	1:A:54:VAL:HG22	1	0.39
(1,641)	1:A:53:SER:H	1:A:54:VAL:HG23	1	0.39
(1,630)	1:B:252:VAL:HG21	1:B:279:ILE:HA	8	0.39
(1,630)	1:B:252:VAL:HG22	1:B:279:ILE:HA	8	0.39
(1,630)	1:B:252:VAL:HG23	1:B:279:ILE:HA	8	0.39
(1,629)	1:B:252:VAL:HG21	1:B:254:VAL:HA	14	0.39
(1,629)	1:B:252:VAL:HG22	1:B:254:VAL:HA	14	0.39
(1,629)	1:B:252:VAL:HG23	1:B:254:VAL:HA	14	0.39
(1,581)	1:A:44:LEU:HD11	1:B:273:PRO:HB3	15	0.39
(1,581)	1:A:44:LEU:HD12	1:B:273:PRO:HB3	15	0.39
(1,581)	1:A:44:LEU:HD13	1:B:273:PRO:HB3	15	0.39
(1,526)	1:A:16:ILE:HB	1:A:29:SER:HA	20	0.39
(1,506)	1:B:254:VAL:HB	1:B:255:TYR:HA	11	0.39
(1,318)	1:A:74:ASN:HB3	1:A:75:GLU:HA	2	0.39
(1,318)	1:A:74:ASN:HB3	1:A:75:GLU:HA	11	0.39
(1,206)	1:B:252:VAL:HB	1:B:253:SER:HA	7	0.39
(1,206)	1:B:252:VAL:HB	1:B:253:SER:HA	15	0.39
(1,205)	1:A:52:VAL:HB	1:A:53:SER:HA	8	0.39
(1,1209)	1:A:27:THR:H	1:A:54:VAL:HB	6	0.39
(1,1151)	1:A:33:LEU:H	1:A:49:GLY:HA3	10	0.39
(1,96)	1:A:70:VAL:HG11	1:A:71:ILE:HA	10	0.38
(1,96)	1:A:70:VAL:HG12	1:A:71:ILE:HA	10	0.38
(1,96)	1:A:70:VAL:HG13	1:A:71:ILE:HA	10	0.38
(1,910)	1:A:103:ASN:H	1:A:124:ILE:HG21	6	0.38
(1,910)	1:A:103:ASN:H	1:A:124:ILE:HG22	6	0.38
(1,910)	1:A:103:ASN:H	1:A:124:ILE:HG23	6	0.38
(1,782)	1:B:315:LEU:H	1:B:316:GLY:HA3	5	0.38
(1,781)	1:A:115:LEU:H	1:A:116:GLY:HA3	3	0.38
(1,781)	1:A:115:LEU:H	1:A:116:GLY:HA3	5	0.38
(1,741)	1:A:124:ILE:H	1:A:124:ILE:HG12	14	0.38
(1,642)	1:B:253:SER:H	1:B:254:VAL:HG21	11	0.38
(1,642)	1:B:253:SER:H	1:B:254:VAL:HG22	11	0.38
(1,642)	1:B:253:SER:H	1:B:254:VAL:HG23	11	0.38
(1,628)	1:A:52:VAL:HG21	1:A:79:ILE:HA	7	0.38
(1,628)	1:A:52:VAL:HG22	1:A:79:ILE:HA	7	0.38

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,628)	1:A:52:VAL:HG23	1:A:79:ILE:HA	7	0.38
(1,618)	1:B:302:ARG:HB2	1:B:303:ASN:HB2	1	0.38
(1,618)	1:B:302:ARG:HB3	1:B:303:ASN:HB2	1	0.38
(1,547)	1:A:20:ASP:HB2	1:A:21:PRO:HB2	17	0.38
(1,499)	1:A:20:ASP:HB2	1:A:23:ARG:HB2	17	0.38
(1,376)	1:B:217:VAL:HB	1:B:227:THR:HB	20	0.38
(1,316)	1:B:232:LEU:HA	1:B:250:GLN:HB2	4	0.38
(1,315)	1:A:32:LEU:HA	1:A:50:GLN:HB2	11	0.38
(1,30)	1:B:232:LEU:HD11	1:B:233:LEU:HA	2	0.38
(1,30)	1:B:232:LEU:HD12	1:B:233:LEU:HA	2	0.38
(1,30)	1:B:232:LEU:HD13	1:B:233:LEU:HA	2	0.38
(1,1216)	1:B:231:SER:H	1:B:252:VAL:HG11	9	0.38
(1,1216)	1:B:231:SER:H	1:B:252:VAL:HG12	9	0.38
(1,1216)	1:B:231:SER:H	1:B:252:VAL:HG13	9	0.38
(1,1108)	1:A:75:GLU:H	1:B:244:LEU:HD11	3	0.38
(1,1108)	1:A:75:GLU:H	1:B:244:LEU:HD12	3	0.38
(1,1108)	1:A:75:GLU:H	1:B:244:LEU:HD13	3	0.38
(1,102)	1:B:293:LEU:HD11	1:B:297:TRP:HA	20	0.38
(1,102)	1:B:293:LEU:HD12	1:B:297:TRP:HA	20	0.38
(1,102)	1:B:293:LEU:HD13	1:B:297:TRP:HA	20	0.38
(1,782)	1:B:315:LEU:H	1:B:316:GLY:HA3	12	0.37
(1,781)	1:A:115:LEU:H	1:A:116:GLY:HA3	13	0.37
(1,630)	1:B:252:VAL:HG21	1:B:279:ILE:HA	12	0.37
(1,630)	1:B:252:VAL:HG22	1:B:279:ILE:HA	12	0.37
(1,630)	1:B:252:VAL:HG23	1:B:279:ILE:HA	12	0.37
(1,477)	1:A:108:PHE:HB2	1:A:110:SER:H	14	0.37
(1,320)	1:B:274:ASN:HB3	1:B:275:GLU:HA	3	0.37
(1,320)	1:B:274:ASN:HB3	1:B:275:GLU:HA	18	0.37
(1,315)	1:A:32:LEU:HA	1:A:50:GLN:HB2	14	0.37
(1,299)	1:A:30:ALA:HB1	1:A:51:TYR:HA	19	0.37
(1,299)	1:A:30:ALA:HB2	1:A:51:TYR:HA	19	0.37
(1,299)	1:A:30:ALA:HB3	1:A:51:TYR:HA	19	0.37
(1,132)	1:A:25:SER:HA	1:A:26:THR:HG21	2	0.37
(1,132)	1:A:25:SER:HA	1:A:26:THR:HG22	2	0.37
(1,132)	1:A:25:SER:HA	1:A:26:THR:HG23	2	0.37
(1,1235)	1:A:18:TRP:HB2	1:A:28:PHE:H	8	0.37
(1,1235)	1:A:18:TRP:HB3	1:A:28:PHE:H	8	0.37
(1,118)	1:B:293:LEU:HD11	1:B:294:LYS:HA	12	0.37
(1,118)	1:B:293:LEU:HD12	1:B:294:LYS:HA	12	0.37
(1,118)	1:B:293:LEU:HD13	1:B:294:LYS:HA	12	0.37
(1,782)	1:B:315:LEU:H	1:B:316:GLY:HA3	6	0.36
(1,782)	1:B:315:LEU:H	1:B:316:GLY:HA3	20	0.36

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,781)	1:A:115:LEU:H	1:A:116:GLY:HA3	6	0.36
(1,742)	1:B:324:ILE:H	1:B:324:ILE:HG12	3	0.36
(1,742)	1:B:324:ILE:H	1:B:324:ILE:HG12	13	0.36
(1,742)	1:B:324:ILE:H	1:B:324:ILE:HG12	20	0.36
(1,741)	1:A:124:ILE:H	1:A:124:ILE:HG12	3	0.36
(1,741)	1:A:124:ILE:H	1:A:124:ILE:HG12	20	0.36
(1,636)	1:B:269:CYS:HB2	1:B:270:VAL:HG11	2	0.36
(1,636)	1:B:269:CYS:HB2	1:B:270:VAL:HG12	2	0.36
(1,636)	1:B:269:CYS:HB2	1:B:270:VAL:HG13	2	0.36
(1,478)	1:B:308:PHE:HB2	1:B:310:SER:H	4	0.36
(1,478)	1:B:308:PHE:HB2	1:B:310:SER:H	14	0.36
(1,460)	1:B:302:ARG:HG3	1:B:305:ASP:HB2	15	0.36
(1,320)	1:B:274:ASN:HB3	1:B:275:GLU:HA	8	0.36
(1,320)	1:B:274:ASN:HB3	1:B:275:GLU:HA	10	0.36
(1,318)	1:A:74:ASN:HB3	1:A:75:GLU:HA	16	0.36
(1,308)	1:B:302:ARG:HG2	1:B:303:ASN:HA	2	0.36
(1,206)	1:B:252:VAL:HB	1:B:253:SER:HA	19	0.36
(1,1260)	1:B:314:GLY:H	1:B:315:LEU:HD21	4	0.36
(1,1260)	1:B:314:GLY:H	1:B:315:LEU:HD22	4	0.36
(1,1260)	1:B:314:GLY:H	1:B:315:LEU:HD23	4	0.36
(1,1234)	1:B:217:VAL:HG11	1:B:228:PHE:H	1	0.36
(1,1234)	1:B:217:VAL:HG12	1:B:228:PHE:H	1	0.36
(1,1234)	1:B:217:VAL:HG13	1:B:228:PHE:H	1	0.36
(1,1214)	1:A:31:SER:H	1:A:52:VAL:HG11	17	0.36
(1,1214)	1:A:31:SER:H	1:A:52:VAL:HG12	17	0.36
(1,1214)	1:A:31:SER:H	1:A:52:VAL:HG13	17	0.36
(1,117)	1:A:93:LEU:HD11	1:A:94:LYS:HA	12	0.36
(1,117)	1:A:93:LEU:HD12	1:A:94:LYS:HA	12	0.36
(1,117)	1:A:93:LEU:HD13	1:A:94:LYS:HA	12	0.36
(1,1065)	1:A:82:VAL:H	1:A:83:ILE:HG12	19	0.36
(1,781)	1:A:115:LEU:H	1:A:116:GLY:HA3	12	0.35
(1,714)	1:A:103:ASN:HB2	1:A:125:VAL:H	8	0.35
(1,477)	1:A:108:PHE:HB2	1:A:110:SER:H	4	0.35
(1,456)	1:A:102:ARG:HB2	1:A:105:ASP:HB2	7	0.35
(1,456)	1:A:102:ARG:HB3	1:A:105:ASP:HB2	7	0.35
(1,308)	1:B:302:ARG:HG2	1:B:303:ASN:HA	17	0.35
(1,307)	1:A:102:ARG:HG2	1:A:103:ASN:HA	2	0.35
(1,1259)	1:A:114:GLY:H	1:A:115:LEU:HD21	4	0.35
(1,1259)	1:A:114:GLY:H	1:A:115:LEU:HD22	4	0.35
(1,1259)	1:A:114:GLY:H	1:A:115:LEU:HD23	4	0.35
(1,1106)	1:B:275:GLU:H	1:B:275:GLU:HG2	19	0.35
(1,106)	1:B:295:ALA:HA	1:B:296:GLU:HG2	14	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,106)	1:B:295:ALA:HA	1:B:296:GLU:HG3	14	0.35
(1,636)	1:B:269:CYS:HB2	1:B:270:VAL:HG11	3	0.34
(1,636)	1:B:269:CYS:HB2	1:B:270:VAL:HG12	3	0.34
(1,636)	1:B:269:CYS:HB2	1:B:270:VAL:HG13	3	0.34
(1,588)	1:B:222:THR:H	1:B:223:ARG:HD3	18	0.34
(1,587)	1:A:22:THR:H	1:A:23:ARG:HD3	20	0.34
(1,460)	1:B:302:ARG:HG3	1:B:305:ASP:HB2	11	0.34
(1,457)	1:A:102:ARG:HG3	1:A:105:ASP:HB2	11	0.34
(1,320)	1:B:274:ASN:HB3	1:B:275:GLU:HA	1	0.34
(1,318)	1:A:74:ASN:HB3	1:A:75:GLU:HA	8	0.34
(1,315)	1:A:32:LEU:HA	1:A:50:GLN:HB2	13	0.34
(1,307)	1:A:102:ARG:HG2	1:A:103:ASN:HA	17	0.34
(1,1233)	1:A:17:VAL:HG11	1:A:28:PHE:H	8	0.34
(1,1233)	1:A:17:VAL:HG12	1:A:28:PHE:H	8	0.34
(1,1233)	1:A:17:VAL:HG13	1:A:28:PHE:H	8	0.34
(1,1223)	1:A:17:VAL:HG11	1:A:29:SER:H	9	0.34
(1,1223)	1:A:17:VAL:HG12	1:A:29:SER:H	9	0.34
(1,1223)	1:A:17:VAL:HG13	1:A:29:SER:H	9	0.34
(1,594)	1:A:49:GLY:H	1:A:50:GLN:HB2	4	0.33
(1,497)	1:A:20:ASP:HB2	1:A:23:ARG:HD3	2	0.33
(1,457)	1:A:102:ARG:HG3	1:A:105:ASP:HB2	20	0.33
(1,320)	1:B:274:ASN:HB3	1:B:275:GLU:HA	2	0.33
(1,320)	1:B:274:ASN:HB3	1:B:275:GLU:HA	15	0.33
(1,320)	1:B:274:ASN:HB3	1:B:275:GLU:HA	20	0.33
(1,318)	1:A:74:ASN:HB3	1:A:75:GLU:HA	15	0.33
(1,306)	1:B:231:SER:HA	1:B:250:GLN:H	12	0.33
(1,257)	1:A:17:VAL:HB	1:A:28:PHE:HA	15	0.33
(1,200)	1:B:272:MET:H	1:B:273:PRO:HA	10	0.33
(1,165)	1:B:247:VAL:HG21	1:B:286:SER:HA	18	0.33
(1,165)	1:B:247:VAL:HG22	1:B:286:SER:HA	18	0.33
(1,165)	1:B:247:VAL:HG23	1:B:286:SER:HA	18	0.33
(1,124)	1:B:293:LEU:HB2	1:B:294:LYS:HA	19	0.33
(1,123)	1:A:93:LEU:HB2	1:A:94:LYS:HA	12	0.33
(1,1153)	1:A:50:GLN:H	1:A:50:GLN:HG2	12	0.33
(1,1153)	1:A:50:GLN:H	1:A:50:GLN:HG3	12	0.33
(1,716)	1:B:303:ASN:HB2	1:B:325:VAL:H	13	0.32
(1,648)	1:B:302:ARG:HG2	1:B:325:VAL:HA	8	0.32
(1,636)	1:B:269:CYS:HB2	1:B:270:VAL:HG11	13	0.32
(1,636)	1:B:269:CYS:HB2	1:B:270:VAL:HG12	13	0.32
(1,636)	1:B:269:CYS:HB2	1:B:270:VAL:HG13	13	0.32
(1,546)	1:B:227:THR:HB	1:B:254:VAL:HB	20	0.32
(1,459)	1:B:302:ARG:HB2	1:B:305:ASP:HB2	7	0.32

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,459)	1:B:302:ARG:HB3	1:B:305:ASP:HB2	7	0.32
(1,315)	1:A:32:LEU:HA	1:A:50:GLN:HB2	17	0.32
(1,160)	1:B:287:ALA:HA	1:B:290:LEU:HD21	16	0.32
(1,160)	1:B:287:ALA:HA	1:B:290:LEU:HD22	16	0.32
(1,160)	1:B:287:ALA:HA	1:B:290:LEU:HD23	16	0.32
(1,1269)	1:A:115:LEU:H	1:A:117:PHE:H	13	0.32
(1,124)	1:B:293:LEU:HB2	1:B:294:LYS:HA	2	0.32
(1,124)	1:B:293:LEU:HB2	1:B:294:LYS:HA	4	0.32
(1,124)	1:B:293:LEU:HB2	1:B:294:LYS:HA	5	0.32
(1,124)	1:B:293:LEU:HB2	1:B:294:LYS:HA	12	0.32
(1,123)	1:A:93:LEU:HB2	1:A:94:LYS:HA	5	0.32
(1,123)	1:A:93:LEU:HB2	1:A:94:LYS:HA	16	0.32
(1,123)	1:A:93:LEU:HB2	1:A:94:LYS:HA	19	0.32
(1,117)	1:A:93:LEU:HD11	1:A:94:LYS:HA	6	0.32
(1,117)	1:A:93:LEU:HD12	1:A:94:LYS:HA	6	0.32
(1,117)	1:A:93:LEU:HD13	1:A:94:LYS:HA	6	0.32
(1,1152)	1:B:233:LEU:H	1:B:249:GLY:HA3	10	0.32
(1,1151)	1:A:33:LEU:H	1:A:49:GLY:HA3	7	0.32
(1,897)	1:A:102:ARG:HG2	1:A:103:ASN:H	2	0.31
(1,647)	1:A:102:ARG:HG2	1:A:125:VAL:HA	13	0.31
(1,608)	1:B:250:GLN:HB2	1:B:251:TYR:HA	19	0.31
(1,400)	1:B:302:ARG:HG2	1:B:324:ILE:HD11	8	0.31
(1,400)	1:B:302:ARG:HG2	1:B:324:ILE:HD12	8	0.31
(1,400)	1:B:302:ARG:HG2	1:B:324:ILE:HD13	8	0.31
(1,320)	1:B:274:ASN:HB3	1:B:275:GLU:HA	12	0.31
(1,318)	1:A:74:ASN:HB3	1:A:75:GLU:HA	20	0.31
(1,297)	1:A:19:SER:HA	1:A:20:ASP:HB3	16	0.31
(1,257)	1:A:17:VAL:HB	1:A:28:PHE:HA	10	0.31
(1,124)	1:B:293:LEU:HB2	1:B:294:LYS:HA	3	0.31
(1,124)	1:B:293:LEU:HB2	1:B:294:LYS:HA	9	0.31
(1,124)	1:B:293:LEU:HB2	1:B:294:LYS:HA	11	0.31
(1,124)	1:B:293:LEU:HB2	1:B:294:LYS:HA	16	0.31
(1,123)	1:A:93:LEU:HB2	1:A:94:LYS:HA	2	0.31
(1,123)	1:A:93:LEU:HB2	1:A:94:LYS:HA	3	0.31
(1,123)	1:A:93:LEU:HB2	1:A:94:LYS:HA	4	0.31
(1,123)	1:A:93:LEU:HB2	1:A:94:LYS:HA	6	0.31
(1,123)	1:A:93:LEU:HB2	1:A:94:LYS:HA	9	0.31
(1,901)	1:A:103:ASN:H	1:A:125:VAL:HG21	4	0.3
(1,901)	1:A:103:ASN:H	1:A:125:VAL:HG22	4	0.3
(1,901)	1:A:103:ASN:H	1:A:125:VAL:HG23	4	0.3
(1,898)	1:B:302:ARG:HG2	1:B:303:ASN:H	2	0.3
(1,778)	1:A:32:LEU:HD11	1:B:316:GLY:H	20	0.3

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,778)	1:A:32:LEU:HD12	1:B:316:GLY:H	20	0.3
(1,778)	1:A:32:LEU:HD13	1:B:316:GLY:H	20	0.3
(1,677)	1:A:90:LEU:HD11	1:A:94:LYS:HG2	13	0.3
(1,677)	1:A:90:LEU:HD12	1:A:94:LYS:HG2	13	0.3
(1,677)	1:A:90:LEU:HD13	1:A:94:LYS:HG2	13	0.3
(1,667)	1:A:88:GLU:HB2	1:A:89:ASN:HB2	3	0.3
(1,667)	1:A:88:GLU:HB2	1:A:89:ASN:HB3	3	0.3
(1,549)	1:B:220:ASP:HB2	1:B:221:PRO:HB2	12	0.3
(1,497)	1:A:20:ASP:HB2	1:A:23:ARG:HD3	16	0.3
(1,318)	1:A:74:ASN:HB3	1:A:75:GLU:HA	1	0.3
(1,318)	1:A:74:ASN:HB3	1:A:75:GLU:HA	17	0.3
(1,316)	1:B:232:LEU:HA	1:B:250:GLN:HB2	5	0.3
(1,297)	1:A:19:SER:HA	1:A:20:ASP:HB3	19	0.3
(1,166)	1:B:244:LEU:HD11	1:B:286:SER:HA	12	0.3
(1,166)	1:B:244:LEU:HD12	1:B:286:SER:HA	12	0.3
(1,166)	1:B:244:LEU:HD13	1:B:286:SER:HA	12	0.3
(1,1267)	1:A:17:VAL:HG11	1:A:19:SER:H	19	0.3
(1,1267)	1:A:17:VAL:HG12	1:A:19:SER:H	19	0.3
(1,1267)	1:A:17:VAL:HG13	1:A:19:SER:H	19	0.3
(1,124)	1:B:293:LEU:HB2	1:B:294:LYS:HA	6	0.3
(1,124)	1:B:293:LEU:HB2	1:B:294:LYS:HA	7	0.3
(1,124)	1:B:293:LEU:HB2	1:B:294:LYS:HA	13	0.3
(1,124)	1:B:293:LEU:HB2	1:B:294:LYS:HA	18	0.3
(1,123)	1:A:93:LEU:HB2	1:A:94:LYS:HA	7	0.3
(1,123)	1:A:93:LEU:HB2	1:A:94:LYS:HA	10	0.3
(1,123)	1:A:93:LEU:HB2	1:A:94:LYS:HA	11	0.3
(1,123)	1:A:93:LEU:HB2	1:A:94:LYS:HA	15	0.3
(1,123)	1:A:93:LEU:HB2	1:A:94:LYS:HA	18	0.3
(1,123)	1:A:93:LEU:HB2	1:A:94:LYS:HA	20	0.3
(1,1226)	1:B:229:SER:H	1:B:252:VAL:HG11	12	0.3
(1,1226)	1:B:229:SER:H	1:B:252:VAL:HG12	12	0.3
(1,1226)	1:B:229:SER:H	1:B:252:VAL:HG13	12	0.3
(1,118)	1:B:293:LEU:HD11	1:B:294:LYS:HA	11	0.3
(1,118)	1:B:293:LEU:HD12	1:B:294:LYS:HA	11	0.3
(1,118)	1:B:293:LEU:HD13	1:B:294:LYS:HA	11	0.3
(1,117)	1:A:93:LEU:HD11	1:A:94:LYS:HA	11	0.3
(1,117)	1:A:93:LEU:HD12	1:A:94:LYS:HA	11	0.3
(1,117)	1:A:93:LEU:HD13	1:A:94:LYS:HA	11	0.3
(1,756)	1:B:320:PRO:HA	1:B:322:ALA:H	20	0.29
(1,587)	1:A:22:THR:H	1:A:23:ARG:HD3	18	0.29
(1,482)	1:B:302:ARG:H	1:B:302:ARG:HD3	4	0.29
(1,477)	1:A:108:PHE:HB2	1:A:110:SER:H	3	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,477)	1:A:108:PHE:HB2	1:A:110:SER:H	11	0.29
(1,457)	1:A:102:ARG:HG3	1:A:105:ASP:HB2	2	0.29
(1,457)	1:A:102:ARG:HG3	1:A:105:ASP:HB2	8	0.29
(1,320)	1:B:274:ASN:HB3	1:B:275:GLU:HA	5	0.29
(1,320)	1:B:274:ASN:HB3	1:B:275:GLU:HA	16	0.29
(1,318)	1:A:74:ASN:HB3	1:A:75:GLU:HA	5	0.29
(1,318)	1:A:74:ASN:HB3	1:A:75:GLU:HA	12	0.29
(1,316)	1:B:232:LEU:HA	1:B:250:GLN:HB2	17	0.29
(1,124)	1:B:293:LEU:HB2	1:B:294:LYS:HA	8	0.29
(1,124)	1:B:293:LEU:HB2	1:B:294:LYS:HA	15	0.29
(1,124)	1:B:293:LEU:HB2	1:B:294:LYS:HA	20	0.29
(1,123)	1:A:93:LEU:HB2	1:A:94:LYS:HA	8	0.29
(1,123)	1:A:93:LEU:HB2	1:A:94:LYS:HA	13	0.29
(1,1223)	1:A:17:VAL:HG11	1:A:29:SER:H	12	0.29
(1,1223)	1:A:17:VAL:HG12	1:A:29:SER:H	12	0.29
(1,1223)	1:A:17:VAL:HG13	1:A:29:SER:H	12	0.29
(1,1155)	1:B:250:GLN:H	1:B:250:GLN:HG2	12	0.29
(1,1155)	1:B:250:GLN:H	1:B:250:GLN:HG3	12	0.29
(1,714)	1:A:103:ASN:HB2	1:A:125:VAL:H	4	0.28
(1,634)	1:A:69:CYS:HB2	1:A:70:VAL:HG11	19	0.28
(1,634)	1:A:69:CYS:HB2	1:A:70:VAL:HG12	19	0.28
(1,634)	1:A:69:CYS:HB2	1:A:70:VAL:HG13	19	0.28
(1,481)	1:A:102:ARG:H	1:A:102:ARG:HD3	4	0.28
(1,478)	1:B:308:PHE:HB2	1:B:310:SER:H	3	0.28
(1,307)	1:A:102:ARG:HG2	1:A:103:ASN:HA	12	0.28
(1,124)	1:B:293:LEU:HB2	1:B:294:LYS:HA	10	0.28
(1,1234)	1:B:217:VAL:HG11	1:B:228:PHE:H	14	0.28
(1,1234)	1:B:217:VAL:HG12	1:B:228:PHE:H	14	0.28
(1,1234)	1:B:217:VAL:HG13	1:B:228:PHE:H	14	0.28
(1,1152)	1:B:233:LEU:H	1:B:249:GLY:HA3	8	0.28
(1,1108)	1:A:75:GLU:H	1:B:244:LEU:HD11	18	0.28
(1,1108)	1:A:75:GLU:H	1:B:244:LEU:HD12	18	0.28
(1,1108)	1:A:75:GLU:H	1:B:244:LEU:HD13	18	0.28
(1,1107)	1:A:44:LEU:HD11	1:B:275:GLU:H	12	0.28
(1,1107)	1:A:44:LEU:HD12	1:B:275:GLU:H	12	0.28
(1,1107)	1:A:44:LEU:HD13	1:B:275:GLU:H	12	0.28
(1,1065)	1:A:82:VAL:H	1:A:83:ILE:HG12	17	0.28
(1,912)	1:B:303:ASN:H	1:B:324:ILE:HG21	6	0.27
(1,912)	1:B:303:ASN:H	1:B:324:ILE:HG22	6	0.27
(1,912)	1:B:303:ASN:H	1:B:324:ILE:HG23	6	0.27
(1,910)	1:A:103:ASN:H	1:A:124:ILE:HG21	8	0.27
(1,910)	1:A:103:ASN:H	1:A:124:ILE:HG22	8	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,910)	1:A:103:ASN:H	1:A:124:ILE:HG23	8	0.27
(1,910)	1:A:103:ASN:H	1:A:124:ILE:HG21	14	0.27
(1,910)	1:A:103:ASN:H	1:A:124:ILE:HG22	14	0.27
(1,910)	1:A:103:ASN:H	1:A:124:ILE:HG23	14	0.27
(1,723)	1:B:303:ASN:HB3	1:B:325:VAL:H	16	0.27
(1,714)	1:A:103:ASN:HB2	1:A:125:VAL:H	13	0.27
(1,634)	1:A:69:CYS:HB2	1:A:70:VAL:HG11	2	0.27
(1,634)	1:A:69:CYS:HB2	1:A:70:VAL:HG12	2	0.27
(1,634)	1:A:69:CYS:HB2	1:A:70:VAL:HG13	2	0.27
(1,588)	1:B:222:THR:H	1:B:223:ARG:HD3	4	0.27
(1,514)	1:A:125:VAL:HB	1:B:205:PRO:HB2	20	0.27
(1,503)	1:A:28:PHE:HA	1:A:54:VAL:HB	19	0.27
(1,498)	1:B:220:ASP:HB2	1:B:223:ARG:HD3	2	0.27
(1,478)	1:B:308:PHE:HB2	1:B:310:SER:H	11	0.27
(1,477)	1:A:108:PHE:HB2	1:A:110:SER:H	5	0.27
(1,308)	1:B:302:ARG:HG2	1:B:303:ASN:HA	8	0.27
(1,164)	1:A:44:LEU:HD11	1:A:86:SER:HA	12	0.27
(1,164)	1:A:44:LEU:HD12	1:A:86:SER:HA	12	0.27
(1,164)	1:A:44:LEU:HD13	1:A:86:SER:HA	12	0.27
(1,1227)	1:A:17:VAL:HA	1:A:28:PHE:H	15	0.27
(1,1152)	1:B:233:LEU:H	1:B:249:GLY:HA3	1	0.27
(1,1152)	1:B:233:LEU:H	1:B:249:GLY:HA3	14	0.27
(1,718)	1:B:302:ARG:HG2	1:B:325:VAL:H	17	0.26
(1,668)	1:B:288:GLU:HB2	1:B:289:ASN:HB2	17	0.26
(1,668)	1:B:288:GLU:HB2	1:B:289:ASN:HB3	17	0.26
(1,667)	1:A:88:GLU:HB2	1:A:89:ASN:HB2	17	0.26
(1,667)	1:A:88:GLU:HB2	1:A:89:ASN:HB3	17	0.26
(1,642)	1:B:253:SER:H	1:B:254:VAL:HG21	20	0.26
(1,642)	1:B:253:SER:H	1:B:254:VAL:HG22	20	0.26
(1,642)	1:B:253:SER:H	1:B:254:VAL:HG23	20	0.26
(1,637)	1:A:119:ASP:HB3	1:A:122:ALA:HB1	20	0.26
(1,637)	1:A:119:ASP:HB3	1:A:122:ALA:HB2	20	0.26
(1,637)	1:A:119:ASP:HB3	1:A:122:ALA:HB3	20	0.26
(1,607)	1:A:50:GLN:HB2	1:A:51:TYR:HA	7	0.26
(1,587)	1:A:22:THR:H	1:A:23:ARG:HD3	4	0.26
(1,585)	1:A:75:GLU:HG3	1:A:76:ASN:H	20	0.26
(1,377)	1:A:17:VAL:HG11	1:A:27:THR:HB	11	0.26
(1,377)	1:A:17:VAL:HG12	1:A:27:THR:HB	11	0.26
(1,377)	1:A:17:VAL:HG13	1:A:27:THR:HB	11	0.26
(1,376)	1:B:217:VAL:HB	1:B:227:THR:HB	14	0.26
(1,359)	1:A:16:ILE:HA	1:A:17:VAL:HG11	20	0.26
(1,359)	1:A:16:ILE:HA	1:A:17:VAL:HG12	20	0.26

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,359)	1:A:16:ILE:HA	1:A:17:VAL:HG13	20	0.26
(1,307)	1:A:102:ARG:HG2	1:A:103:ASN:HA	13	0.26
(1,259)	1:B:217:VAL:HB	1:B:228:PHE:HA	12	0.26
(1,163)	1:A:47:VAL:HG21	1:A:86:SER:HA	7	0.26
(1,163)	1:A:47:VAL:HG22	1:A:86:SER:HA	7	0.26
(1,163)	1:A:47:VAL:HG23	1:A:86:SER:HA	7	0.26
(1,1299)	1:B:297:TRP:HB2	1:B:297:TRP:HE1	1	0.26
(1,1267)	1:A:17:VAL:HG11	1:A:19:SER:H	15	0.26
(1,1267)	1:A:17:VAL:HG12	1:A:19:SER:H	15	0.26
(1,1267)	1:A:17:VAL:HG13	1:A:19:SER:H	15	0.26
(1,1151)	1:A:33:LEU:H	1:A:49:GLY:HA3	14	0.26
(1,96)	1:A:70:VAL:HG11	1:A:71:ILE:HA	4	0.25
(1,96)	1:A:70:VAL:HG12	1:A:71:ILE:HA	4	0.25
(1,96)	1:A:70:VAL:HG13	1:A:71:ILE:HA	4	0.25
(1,931)	1:B:232:LEU:HD11	1:B:233:LEU:H	5	0.25
(1,931)	1:B:232:LEU:HD12	1:B:233:LEU:H	5	0.25
(1,931)	1:B:232:LEU:HD13	1:B:233:LEU:H	5	0.25
(1,901)	1:A:103:ASN:H	1:A:125:VAL:HG21	16	0.25
(1,901)	1:A:103:ASN:H	1:A:125:VAL:HG22	16	0.25
(1,901)	1:A:103:ASN:H	1:A:125:VAL:HG23	16	0.25
(1,690)	1:B:208:PRO:HG2	1:B:218:TRP:HB2	14	0.25
(1,690)	1:B:208:PRO:HG2	1:B:218:TRP:HB3	14	0.25
(1,690)	1:B:208:PRO:HG3	1:B:218:TRP:HB2	14	0.25
(1,690)	1:B:208:PRO:HG3	1:B:218:TRP:HB3	14	0.25
(1,668)	1:B:288:GLU:HB2	1:B:289:ASN:HB2	3	0.25
(1,668)	1:B:288:GLU:HB2	1:B:289:ASN:HB3	3	0.25
(1,610)	1:B:249:GLY:HA3	1:B:250:GLN:HB2	12	0.25
(1,608)	1:B:250:GLN:HB2	1:B:251:TYR:HA	6	0.25
(1,597)	1:B:249:GLY:H	1:B:250:GLN:HB2	14	0.25
(1,594)	1:A:49:GLY:H	1:A:50:GLN:HB2	5	0.25
(1,586)	1:B:275:GLU:HG3	1:B:276:ASN:H	18	0.25
(1,586)	1:B:275:GLU:HG3	1:B:276:ASN:H	20	0.25
(1,585)	1:A:75:GLU:HG3	1:A:76:ASN:H	18	0.25
(1,550)	1:B:269:CYS:HB3	1:B:270:VAL:HB	2	0.25
(1,498)	1:B:220:ASP:HB2	1:B:223:ARG:HD3	19	0.25
(1,308)	1:B:302:ARG:HG2	1:B:303:ASN:HA	12	0.25
(1,301)	1:B:230:ALA:HB1	1:B:251:TYR:HA	12	0.25
(1,301)	1:B:230:ALA:HB2	1:B:251:TYR:HA	12	0.25
(1,301)	1:B:230:ALA:HB3	1:B:251:TYR:HA	12	0.25
(1,298)	1:B:219:SER:HA	1:B:220:ASP:HB3	1	0.25
(1,297)	1:A:19:SER:HA	1:A:20:ASP:HB3	12	0.25
(1,1297)	1:A:97:TRP:HB2	1:A:97:TRP:HE1	1	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1235)	1:A:18:TRP:HB2	1:A:28:PHE:H	17	0.25
(1,1235)	1:A:18:TRP:HB3	1:A:28:PHE:H	17	0.25
(1,1202)	1:A:31:SER:H	1:A:50:GLN:H	19	0.25
(1,117)	1:A:93:LEU:HD11	1:A:94:LYS:HA	16	0.25
(1,117)	1:A:93:LEU:HD12	1:A:94:LYS:HA	16	0.25
(1,117)	1:A:93:LEU:HD13	1:A:94:LYS:HA	16	0.25
(1,1152)	1:B:233:LEU:H	1:B:249:GLY:HA3	7	0.25
(1,1151)	1:A:33:LEU:H	1:A:49:GLY:HA3	8	0.25
(1,929)	1:A:32:LEU:HD11	1:A:33:LEU:H	5	0.24
(1,929)	1:A:32:LEU:HD12	1:A:33:LEU:H	5	0.24
(1,929)	1:A:32:LEU:HD13	1:A:33:LEU:H	5	0.24
(1,912)	1:B:303:ASN:H	1:B:324:ILE:HG21	14	0.24
(1,912)	1:B:303:ASN:H	1:B:324:ILE:HG22	14	0.24
(1,912)	1:B:303:ASN:H	1:B:324:ILE:HG23	14	0.24
(1,608)	1:B:250:GLN:HB2	1:B:251:TYR:HA	15	0.24
(1,607)	1:A:50:GLN:HB2	1:A:51:TYR:HA	12	0.24
(1,607)	1:A:50:GLN:HB2	1:A:51:TYR:HA	15	0.24
(1,581)	1:A:44:LEU:HD11	1:B:273:PRO:HB3	20	0.24
(1,581)	1:A:44:LEU:HD12	1:B:273:PRO:HB3	20	0.24
(1,581)	1:A:44:LEU:HD13	1:B:273:PRO:HB3	20	0.24
(1,504)	1:A:54:VAL:HB	1:A:55:TYR:HA	1	0.24
(1,50)	1:B:303:ASN:HA	1:B:306:THR:HG1	6	0.24
(1,481)	1:A:102:ARG:H	1:A:102:ARG:HD3	15	0.24
(1,478)	1:B:308:PHE:HB2	1:B:310:SER:H	9	0.24
(1,477)	1:A:108:PHE:HB2	1:A:110:SER:H	9	0.24
(1,361)	1:B:216:ILE:HA	1:B:217:VAL:HG11	20	0.24
(1,361)	1:B:216:ILE:HA	1:B:217:VAL:HG12	20	0.24
(1,361)	1:B:216:ILE:HA	1:B:217:VAL:HG13	20	0.24
(1,320)	1:B:274:ASN:HB3	1:B:275:GLU:HA	6	0.24
(1,198)	1:A:72:MET:H	1:A:73:PRO:HA	3	0.24
(1,1312)	1:B:232:LEU:HD11	1:B:234:ARG:H	13	0.24
(1,1312)	1:B:232:LEU:HD12	1:B:234:ARG:H	13	0.24
(1,1312)	1:B:232:LEU:HD13	1:B:234:ARG:H	13	0.24
(1,1267)	1:A:17:VAL:HG11	1:A:19:SER:H	13	0.24
(1,1267)	1:A:17:VAL:HG12	1:A:19:SER:H	13	0.24
(1,1267)	1:A:17:VAL:HG13	1:A:19:SER:H	13	0.24
(1,1151)	1:A:33:LEU:H	1:A:49:GLY:HA3	1	0.24
(1,1085)	1:A:78:SER:H	1:A:79:ILE:HG12	6	0.24
(1,1036)	1:A:84:SER:H	1:B:279:ILE:HD11	19	0.24
(1,1036)	1:A:84:SER:H	1:B:279:ILE:HD12	19	0.24
(1,1036)	1:A:84:SER:H	1:B:279:ILE:HD13	19	0.24
(1,844)	1:B:306:THR:H	1:B:306:THR:HG1	6	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,717)	1:A:102:ARG:HG2	1:A:125:VAL:H	20	0.23
(1,716)	1:B:303:ASN:HB2	1:B:325:VAL:H	4	0.23
(1,632)	1:B:302:ARG:HD3	1:B:325:VAL:HG21	17	0.23
(1,632)	1:B:302:ARG:HD3	1:B:325:VAL:HG22	17	0.23
(1,632)	1:B:302:ARG:HD3	1:B:325:VAL:HG23	17	0.23
(1,607)	1:A:50:GLN:HB2	1:A:51:TYR:HA	19	0.23
(1,597)	1:B:249:GLY:H	1:B:250:GLN:HB2	20	0.23
(1,548)	1:A:69:CYS:HB3	1:A:70:VAL:HB	1	0.23
(1,318)	1:A:74:ASN:HB3	1:A:75:GLU:HA	6	0.23
(1,200)	1:B:272:MET:H	1:B:273:PRO:HA	14	0.23
(1,165)	1:B:247:VAL:HG21	1:B:286:SER:HA	14	0.23
(1,165)	1:B:247:VAL:HG22	1:B:286:SER:HA	14	0.23
(1,165)	1:B:247:VAL:HG23	1:B:286:SER:HA	14	0.23
(1,1311)	1:A:32:LEU:HD11	1:A:34:ARG:H	3	0.23
(1,1311)	1:A:32:LEU:HD12	1:A:34:ARG:H	3	0.23
(1,1311)	1:A:32:LEU:HD13	1:A:34:ARG:H	3	0.23
(1,1249)	1:A:70:VAL:HG11	1:A:72:MET:H	2	0.23
(1,1249)	1:A:70:VAL:HG12	1:A:72:MET:H	2	0.23
(1,1249)	1:A:70:VAL:HG13	1:A:72:MET:H	2	0.23
(1,124)	1:B:293:LEU:HB2	1:B:294:LYS:HA	14	0.23
(1,123)	1:A:93:LEU:HB2	1:A:94:LYS:HA	14	0.23
(1,1189)	1:A:16:ILE:HB	1:A:17:VAL:H	20	0.23
(1,897)	1:A:102:ARG:HG2	1:A:103:ASN:H	12	0.22
(1,851)	1:A:97:TRP:HE1	1:B:305:ASP:H	4	0.22
(1,716)	1:B:303:ASN:HB2	1:B:325:VAL:H	8	0.22
(1,714)	1:A:103:ASN:HB2	1:A:125:VAL:H	15	0.22
(1,639)	1:A:119:ASP:H	1:A:121:THR:HG21	13	0.22
(1,639)	1:A:119:ASP:H	1:A:121:THR:HG22	13	0.22
(1,639)	1:A:119:ASP:H	1:A:121:THR:HG23	13	0.22
(1,456)	1:A:102:ARG:HB2	1:A:105:ASP:HB2	18	0.22
(1,456)	1:A:102:ARG:HB3	1:A:105:ASP:HB2	18	0.22
(1,400)	1:B:302:ARG:HG2	1:B:324:ILE:HD11	12	0.22
(1,400)	1:B:302:ARG:HG2	1:B:324:ILE:HD12	12	0.22
(1,400)	1:B:302:ARG:HG2	1:B:324:ILE:HD13	12	0.22
(1,307)	1:A:102:ARG:HG2	1:A:103:ASN:HA	20	0.22
(1,1312)	1:B:232:LEU:HD11	1:B:234:ARG:H	3	0.22
(1,1312)	1:B:232:LEU:HD12	1:B:234:ARG:H	3	0.22
(1,1312)	1:B:232:LEU:HD13	1:B:234:ARG:H	3	0.22
(1,1296)	1:A:97:TRP:HE1	1:B:305:ASP:HA	6	0.22
(1,1235)	1:A:18:TRP:HB2	1:A:28:PHE:H	7	0.22
(1,1235)	1:A:18:TRP:HB3	1:A:28:PHE:H	7	0.22
(1,1235)	1:A:18:TRP:HB2	1:A:28:PHE:H	20	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1235)	1:A:18:TRP:HB3	1:A:28:PHE:H	20	0.22
(1,118)	1:B:293:LEU:HD11	1:B:294:LYS:HA	5	0.22
(1,118)	1:B:293:LEU:HD12	1:B:294:LYS:HA	5	0.22
(1,118)	1:B:293:LEU:HD13	1:B:294:LYS:HA	5	0.22
(1,1108)	1:A:75:GLU:H	1:B:244:LEU:HD11	12	0.22
(1,1108)	1:A:75:GLU:H	1:B:244:LEU:HD12	12	0.22
(1,1108)	1:A:75:GLU:H	1:B:244:LEU:HD13	12	0.22
(1,904)	1:B:303:ASN:H	1:B:325:VAL:HG21	6	0.21
(1,904)	1:B:303:ASN:H	1:B:325:VAL:HG22	6	0.21
(1,904)	1:B:303:ASN:H	1:B:325:VAL:HG23	6	0.21
(1,904)	1:B:303:ASN:H	1:B:325:VAL:HG21	13	0.21
(1,904)	1:B:303:ASN:H	1:B:325:VAL:HG22	13	0.21
(1,904)	1:B:303:ASN:H	1:B:325:VAL:HG23	13	0.21
(1,898)	1:B:302:ARG:HG2	1:B:303:ASN:H	17	0.21
(1,897)	1:A:102:ARG:HG2	1:A:103:ASN:H	17	0.21
(1,774)	1:B:315:LEU:HD21	1:B:317:PHE:H	2	0.21
(1,774)	1:B:315:LEU:HD22	1:B:317:PHE:H	2	0.21
(1,774)	1:B:315:LEU:HD23	1:B:317:PHE:H	2	0.21
(1,714)	1:A:103:ASN:HB2	1:A:125:VAL:H	11	0.21
(1,690)	1:B:208:PRO:HG2	1:B:218:TRP:HB2	17	0.21
(1,690)	1:B:208:PRO:HG2	1:B:218:TRP:HB3	17	0.21
(1,690)	1:B:208:PRO:HG3	1:B:218:TRP:HB2	17	0.21
(1,690)	1:B:208:PRO:HG3	1:B:218:TRP:HB3	17	0.21
(1,650)	1:B:314:GLY:HA3	1:B:315:LEU:HG	20	0.21
(1,608)	1:B:250:GLN:HB2	1:B:251:TYR:HA	18	0.21
(1,607)	1:A:50:GLN:HB2	1:A:51:TYR:HA	18	0.21
(1,505)	1:B:228:PHE:HA	1:B:254:VAL:HB	11	0.21
(1,379)	1:B:217:VAL:HG11	1:B:227:THR:HB	9	0.21
(1,379)	1:B:217:VAL:HG12	1:B:227:THR:HB	9	0.21
(1,379)	1:B:217:VAL:HG13	1:B:227:THR:HB	9	0.21
(1,377)	1:A:17:VAL:HG11	1:A:27:THR:HB	17	0.21
(1,377)	1:A:17:VAL:HG12	1:A:27:THR:HB	17	0.21
(1,377)	1:A:17:VAL:HG13	1:A:27:THR:HB	17	0.21
(1,318)	1:A:74:ASN:HB3	1:A:75:GLU:HA	19	0.21
(1,260)	1:B:228:PHE:HA	1:B:252:VAL:HB	6	0.21
(1,257)	1:A:17:VAL:HB	1:A:28:PHE:HA	9	0.21
(1,117)	1:A:93:LEU:HD11	1:A:94:LYS:HA	5	0.21
(1,117)	1:A:93:LEU:HD12	1:A:94:LYS:HA	5	0.21
(1,117)	1:A:93:LEU:HD13	1:A:94:LYS:HA	5	0.21
(1,920)	1:B:301:LYS:H	1:B:302:ARG:HB2	1	0.2
(1,920)	1:B:301:LYS:H	1:B:302:ARG:HB3	1	0.2
(1,912)	1:B:303:ASN:H	1:B:324:ILE:HG21	16	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,912)	1:B:303:ASN:H	1:B:324:ILE:HG22	16	0.2
(1,912)	1:B:303:ASN:H	1:B:324:ILE:HG23	16	0.2
(1,904)	1:B:303:ASN:H	1:B:325:VAL:HG21	10	0.2
(1,904)	1:B:303:ASN:H	1:B:325:VAL:HG22	10	0.2
(1,904)	1:B:303:ASN:H	1:B:325:VAL:HG23	10	0.2
(1,902)	1:A:103:ASN:H	1:A:124:ILE:HG12	16	0.2
(1,901)	1:A:103:ASN:H	1:A:125:VAL:HG21	8	0.2
(1,901)	1:A:103:ASN:H	1:A:125:VAL:HG22	8	0.2
(1,901)	1:A:103:ASN:H	1:A:125:VAL:HG23	8	0.2
(1,897)	1:A:102:ARG:HG2	1:A:103:ASN:H	13	0.2
(1,754)	1:B:306:THR:HG21	1:B:323:ALA:H	6	0.2
(1,754)	1:B:306:THR:HG22	1:B:323:ALA:H	6	0.2
(1,754)	1:B:306:THR:HG23	1:B:323:ALA:H	6	0.2
(1,716)	1:B:303:ASN:HB2	1:B:325:VAL:H	17	0.2
(1,588)	1:B:222:THR:H	1:B:223:ARG:HD3	20	0.2
(1,586)	1:B:275:GLU:HG3	1:B:276:ASN:H	7	0.2
(1,585)	1:A:75:GLU:HG3	1:A:76:ASN:H	3	0.2
(1,56)	1:B:303:ASN:HA	1:B:324:ILE:HA	18	0.2
(1,55)	1:A:103:ASN:HA	1:A:124:ILE:HA	18	0.2
(1,548)	1:A:69:CYS:HB3	1:A:70:VAL:HB	13	0.2
(1,504)	1:A:54:VAL:HB	1:A:55:TYR:HA	6	0.2
(1,478)	1:B:308:PHE:HB2	1:B:310:SER:H	10	0.2
(1,477)	1:A:108:PHE:HB2	1:A:110:SER:H	13	0.2
(1,438)	1:A:69:CYS:HA	1:A:70:VAL:HG11	7	0.2
(1,438)	1:A:69:CYS:HA	1:A:70:VAL:HG12	7	0.2
(1,438)	1:A:69:CYS:HA	1:A:70:VAL:HG13	7	0.2
(1,315)	1:A:32:LEU:HA	1:A:50:GLN:HB2	6	0.2
(1,259)	1:B:217:VAL:HB	1:B:228:PHE:HA	1	0.2
(1,257)	1:A:17:VAL:HB	1:A:28:PHE:HA	8	0.2
(1,200)	1:B:272:MET:H	1:B:273:PRO:HA	18	0.2
(1,199)	1:B:259:ALA:H	1:B:273:PRO:HA	18	0.2
(1,198)	1:A:72:MET:H	1:A:73:PRO:HA	2	0.2
(1,172)	1:A:48:SER:HA	1:A:83:ILE:HA	19	0.2
(1,1268)	1:B:217:VAL:HG11	1:B:219:SER:H	20	0.2
(1,1268)	1:B:217:VAL:HG12	1:B:219:SER:H	20	0.2
(1,1268)	1:B:217:VAL:HG13	1:B:219:SER:H	20	0.2
(1,1267)	1:A:17:VAL:HG11	1:A:19:SER:H	10	0.2
(1,1267)	1:A:17:VAL:HG12	1:A:19:SER:H	10	0.2
(1,1267)	1:A:17:VAL:HG13	1:A:19:SER:H	10	0.2
(1,1236)	1:B:218:TRP:HB2	1:B:228:PHE:H	20	0.2
(1,1236)	1:B:218:TRP:HB3	1:B:228:PHE:H	20	0.2
(1,1141)	1:A:50:GLN:H	1:A:83:ILE:H	17	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1085)	1:A:78:SER:H	1:A:79:ILE:HG12	17	0.2
(1,1036)	1:A:84:SER:H	1:B:279:ILE:HD11	12	0.2
(1,1036)	1:A:84:SER:H	1:B:279:ILE:HD12	12	0.2
(1,1036)	1:A:84:SER:H	1:B:279:ILE:HD13	12	0.2
(1,901)	1:A:103:ASN:H	1:A:125:VAL:HG21	10	0.19
(1,901)	1:A:103:ASN:H	1:A:125:VAL:HG22	10	0.19
(1,901)	1:A:103:ASN:H	1:A:125:VAL:HG23	10	0.19
(1,716)	1:B:303:ASN:HB2	1:B:325:VAL:H	11	0.19
(1,716)	1:B:303:ASN:HB2	1:B:325:VAL:H	15	0.19
(1,714)	1:A:103:ASN:HB2	1:A:125:VAL:H	17	0.19
(1,608)	1:B:250:GLN:HB2	1:B:251:TYR:HA	1	0.19
(1,607)	1:A:50:GLN:HB2	1:A:51:TYR:HA	6	0.19
(1,585)	1:A:75:GLU:HG3	1:A:76:ASN:H	7	0.19
(1,56)	1:B:303:ASN:HA	1:B:324:ILE:HA	9	0.19
(1,55)	1:A:103:ASN:HA	1:A:124:ILE:HA	11	0.19
(1,506)	1:B:254:VAL:HB	1:B:255:TYR:HA	20	0.19
(1,459)	1:B:302:ARG:HB2	1:B:305:ASP:HB2	18	0.19
(1,459)	1:B:302:ARG:HB3	1:B:305:ASP:HB2	18	0.19
(1,380)	1:B:227:THR:HB	1:B:254:VAL:HG21	17	0.19
(1,380)	1:B:227:THR:HB	1:B:254:VAL:HG22	17	0.19
(1,380)	1:B:227:THR:HB	1:B:254:VAL:HG23	17	0.19
(1,377)	1:A:17:VAL:HG11	1:A:27:THR:HB	1	0.19
(1,377)	1:A:17:VAL:HG12	1:A:27:THR:HB	1	0.19
(1,377)	1:A:17:VAL:HG13	1:A:27:THR:HB	1	0.19
(1,317)	1:A:75:GLU:HA	1:A:76:ASN:HB3	14	0.19
(1,316)	1:B:232:LEU:HA	1:B:250:GLN:HB2	19	0.19
(1,296)	1:B:219:SER:HA	1:B:227:THR:HG21	8	0.19
(1,296)	1:B:219:SER:HA	1:B:227:THR:HG22	8	0.19
(1,296)	1:B:219:SER:HA	1:B:227:THR:HG23	8	0.19
(1,257)	1:A:17:VAL:HB	1:A:28:PHE:HA	12	0.19
(1,200)	1:B:272:MET:H	1:B:273:PRO:HA	1	0.19
(1,198)	1:A:72:MET:H	1:A:73:PRO:HA	9	0.19
(1,172)	1:A:48:SER:HA	1:A:83:ILE:HA	12	0.19
(1,164)	1:A:44:LEU:HD11	1:A:86:SER:HA	3	0.19
(1,164)	1:A:44:LEU:HD12	1:A:86:SER:HA	3	0.19
(1,164)	1:A:44:LEU:HD13	1:A:86:SER:HA	3	0.19
(1,160)	1:B:287:ALA:HA	1:B:290:LEU:HD21	17	0.19
(1,160)	1:B:287:ALA:HA	1:B:290:LEU:HD22	17	0.19
(1,160)	1:B:287:ALA:HA	1:B:290:LEU:HD23	17	0.19
(1,1312)	1:B:232:LEU:HD11	1:B:234:ARG:H	2	0.19
(1,1312)	1:B:232:LEU:HD12	1:B:234:ARG:H	2	0.19
(1,1312)	1:B:232:LEU:HD13	1:B:234:ARG:H	2	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1234)	1:B:217:VAL:HG11	1:B:228:PHE:H	4	0.19
(1,1234)	1:B:217:VAL:HG12	1:B:228:PHE:H	4	0.19
(1,1234)	1:B:217:VAL:HG13	1:B:228:PHE:H	4	0.19
(1,1233)	1:A:17:VAL:HG11	1:A:28:PHE:H	16	0.19
(1,1233)	1:A:17:VAL:HG12	1:A:28:PHE:H	16	0.19
(1,1233)	1:A:17:VAL:HG13	1:A:28:PHE:H	16	0.19
(1,1224)	1:A:29:SER:H	1:A:52:VAL:HG11	19	0.19
(1,1224)	1:A:29:SER:H	1:A:52:VAL:HG12	19	0.19
(1,1224)	1:A:29:SER:H	1:A:52:VAL:HG13	19	0.19
(1,1152)	1:B:233:LEU:H	1:B:249:GLY:HA3	5	0.19
(1,1087)	1:B:278:SER:H	1:B:279:ILE:HG12	6	0.19
(1,912)	1:B:303:ASN:H	1:B:324:ILE:HG21	20	0.18
(1,912)	1:B:303:ASN:H	1:B:324:ILE:HG22	20	0.18
(1,912)	1:B:303:ASN:H	1:B:324:ILE:HG23	20	0.18
(1,901)	1:A:103:ASN:H	1:A:125:VAL:HG21	6	0.18
(1,901)	1:A:103:ASN:H	1:A:125:VAL:HG22	6	0.18
(1,901)	1:A:103:ASN:H	1:A:125:VAL:HG23	6	0.18
(1,898)	1:B:302:ARG:HG2	1:B:303:ASN:H	12	0.18
(1,852)	1:A:105:ASP:H	1:B:297:TRP:HE1	15	0.18
(1,797)	1:A:20:ASP:H	1:A:24:LEU:H	17	0.18
(1,650)	1:B:314:GLY:HA3	1:B:315:LEU:HG	5	0.18
(1,649)	1:A:114:GLY:HA3	1:A:115:LEU:HG	5	0.18
(1,649)	1:A:114:GLY:HA3	1:A:115:LEU:HG	13	0.18
(1,608)	1:B:250:GLN:HB2	1:B:251:TYR:HA	8	0.18
(1,608)	1:B:250:GLN:HB2	1:B:251:TYR:HA	10	0.18
(1,608)	1:B:250:GLN:HB2	1:B:251:TYR:HA	17	0.18
(1,607)	1:A:50:GLN:HB2	1:A:51:TYR:HA	8	0.18
(1,607)	1:A:50:GLN:HB2	1:A:51:TYR:HA	10	0.18
(1,594)	1:A:49:GLY:H	1:A:50:GLN:HB2	13	0.18
(1,554)	1:B:224:LEU:HB3	1:B:226:THR:HA	10	0.18
(1,550)	1:B:269:CYS:HB3	1:B:270:VAL:HB	19	0.18
(1,55)	1:A:103:ASN:HA	1:A:124:ILE:HA	9	0.18
(1,548)	1:A:69:CYS:HB3	1:A:70:VAL:HB	14	0.18
(1,548)	1:A:69:CYS:HB3	1:A:70:VAL:HB	18	0.18
(1,477)	1:A:108:PHE:HB2	1:A:110:SER:H	10	0.18
(1,375)	1:A:17:VAL:HB	1:A:27:THR:HB	11	0.18
(1,354)	1:B:217:VAL:HG11	1:B:218:TRP:HA	15	0.18
(1,354)	1:B:217:VAL:HG12	1:B:218:TRP:HA	15	0.18
(1,354)	1:B:217:VAL:HG13	1:B:218:TRP:HA	15	0.18
(1,353)	1:A:17:VAL:HG11	1:A:18:TRP:HA	5	0.18
(1,353)	1:A:17:VAL:HG12	1:A:18:TRP:HA	5	0.18
(1,353)	1:A:17:VAL:HG13	1:A:18:TRP:HA	5	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,273)	1:B:220:ASP:HA	1:B:224:LEU:H	15	0.18
(1,166)	1:B:244:LEU:HD11	1:B:286:SER:HA	3	0.18
(1,166)	1:B:244:LEU:HD12	1:B:286:SER:HA	3	0.18
(1,166)	1:B:244:LEU:HD13	1:B:286:SER:HA	3	0.18
(1,124)	1:B:293:LEU:HB2	1:B:294:LYS:HA	17	0.18
(1,1155)	1:B:250:GLN:H	1:B:250:GLN:HG2	1	0.18
(1,1155)	1:B:250:GLN:H	1:B:250:GLN:HG3	1	0.18
(1,901)	1:A:103:ASN:H	1:A:125:VAL:HG21	11	0.17
(1,901)	1:A:103:ASN:H	1:A:125:VAL:HG22	11	0.17
(1,901)	1:A:103:ASN:H	1:A:125:VAL:HG23	11	0.17
(1,898)	1:B:302:ARG:HG2	1:B:303:ASN:H	8	0.17
(1,800)	1:B:312:ASN:H	1:B:315:LEU:HD21	10	0.17
(1,800)	1:B:312:ASN:H	1:B:315:LEU:HD22	10	0.17
(1,800)	1:B:312:ASN:H	1:B:315:LEU:HD23	10	0.17
(1,714)	1:A:103:ASN:HB2	1:A:125:VAL:H	5	0.17
(1,680)	1:B:293:LEU:HD11	1:B:294:LYS:HG2	11	0.17
(1,680)	1:B:293:LEU:HD12	1:B:294:LYS:HG2	11	0.17
(1,680)	1:B:293:LEU:HD13	1:B:294:LYS:HG2	11	0.17
(1,678)	1:A:93:LEU:HD11	1:A:94:LYS:HG2	11	0.17
(1,678)	1:A:93:LEU:HD12	1:A:94:LYS:HG2	11	0.17
(1,678)	1:A:93:LEU:HD13	1:A:94:LYS:HG2	11	0.17
(1,674)	1:B:287:ALA:HB1	1:B:288:GLU:HB3	3	0.17
(1,674)	1:B:287:ALA:HB2	1:B:288:GLU:HB3	3	0.17
(1,674)	1:B:287:ALA:HB3	1:B:288:GLU:HB3	3	0.17
(1,649)	1:A:114:GLY:HA3	1:A:115:LEU:HG	11	0.17
(1,647)	1:A:102:ARG:HG2	1:A:125:VAL:HA	16	0.17
(1,636)	1:B:269:CYS:HB2	1:B:270:VAL:HG11	19	0.17
(1,636)	1:B:269:CYS:HB2	1:B:270:VAL:HG12	19	0.17
(1,636)	1:B:269:CYS:HB2	1:B:270:VAL:HG13	19	0.17
(1,608)	1:B:250:GLN:HB2	1:B:251:TYR:HA	7	0.17
(1,607)	1:A:50:GLN:HB2	1:A:51:TYR:HA	11	0.17
(1,604)	1:B:259:ALA:H	1:B:273:PRO:HB2	10	0.17
(1,482)	1:B:302:ARG:H	1:B:302:ARG:HD3	15	0.17
(1,478)	1:B:308:PHE:HB2	1:B:310:SER:H	13	0.17
(1,352)	1:B:208:PRO:HA	1:B:218:TRP:HA	8	0.17
(1,327)	1:B:302:ARG:HB2	1:B:326:SER:HA	1	0.17
(1,327)	1:B:302:ARG:HB3	1:B:326:SER:HA	1	0.17
(1,319)	1:B:275:GLU:HA	1:B:276:ASN:HB3	14	0.17
(1,216)	1:B:251:TYR:HA	1:B:252:VAL:HB	14	0.17
(1,198)	1:A:72:MET:H	1:A:73:PRO:HA	20	0.17
(1,118)	1:B:293:LEU:HD11	1:B:294:LYS:HA	6	0.17
(1,118)	1:B:293:LEU:HD12	1:B:294:LYS:HA	6	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,118)	1:B:293:LEU:HD13	1:B:294:LYS:HA	6	0.17
(1,118)	1:B:293:LEU:HD11	1:B:294:LYS:HA	15	0.17
(1,118)	1:B:293:LEU:HD12	1:B:294:LYS:HA	15	0.17
(1,118)	1:B:293:LEU:HD13	1:B:294:LYS:HA	15	0.17
(1,1161)	1:A:93:LEU:H	1:A:96:GLU:H	4	0.17
(1,1153)	1:A:50:GLN:H	1:A:50:GLN:HG2	1	0.17
(1,1153)	1:A:50:GLN:H	1:A:50:GLN:HG3	1	0.17
(1,1126)	1:B:230:ALA:HA	1:B:252:VAL:H	12	0.17
(1,1065)	1:A:82:VAL:H	1:A:83:ILE:HG12	18	0.17
(1,1034)	1:A:79:ILE:HD11	1:B:284:SER:H	19	0.17
(1,1034)	1:A:79:ILE:HD12	1:B:284:SER:H	19	0.17
(1,1034)	1:A:79:ILE:HD13	1:B:284:SER:H	19	0.17
(1,100)	1:B:294:LYS:HA	1:B:297:TRP:HA	18	0.17
(1,98)	1:B:270:VAL:HG11	1:B:271:ILE:HA	17	0.16
(1,98)	1:B:270:VAL:HG12	1:B:271:ILE:HA	17	0.16
(1,98)	1:B:270:VAL:HG13	1:B:271:ILE:HA	17	0.16
(1,919)	1:A:101:LYS:H	1:A:102:ARG:HB2	16	0.16
(1,919)	1:A:101:LYS:H	1:A:102:ARG:HB3	16	0.16
(1,773)	1:A:115:LEU:HD21	1:A:117:PHE:H	2	0.16
(1,773)	1:A:115:LEU:HD22	1:A:117:PHE:H	2	0.16
(1,773)	1:A:115:LEU:HD23	1:A:117:PHE:H	2	0.16
(1,754)	1:B:306:THR:HG21	1:B:323:ALA:H	13	0.16
(1,754)	1:B:306:THR:HG22	1:B:323:ALA:H	13	0.16
(1,754)	1:B:306:THR:HG23	1:B:323:ALA:H	13	0.16
(1,753)	1:A:106:THR:HG21	1:A:123:ALA:H	4	0.16
(1,753)	1:A:106:THR:HG22	1:A:123:ALA:H	4	0.16
(1,753)	1:A:106:THR:HG23	1:A:123:ALA:H	4	0.16
(1,717)	1:A:102:ARG:HG2	1:A:125:VAL:H	17	0.16
(1,716)	1:B:303:ASN:HB2	1:B:325:VAL:H	2	0.16
(1,680)	1:B:293:LEU:HD11	1:B:294:LYS:HG2	12	0.16
(1,680)	1:B:293:LEU:HD12	1:B:294:LYS:HG2	12	0.16
(1,680)	1:B:293:LEU:HD13	1:B:294:LYS:HG2	12	0.16
(1,673)	1:A:87:ALA:HB1	1:A:88:GLU:HB3	3	0.16
(1,673)	1:A:87:ALA:HB2	1:A:88:GLU:HB3	3	0.16
(1,673)	1:A:87:ALA:HB3	1:A:88:GLU:HB3	3	0.16
(1,647)	1:A:102:ARG:HG2	1:A:125:VAL:HA	2	0.16
(1,634)	1:A:69:CYS:HB2	1:A:70:VAL:HG11	14	0.16
(1,634)	1:A:69:CYS:HB2	1:A:70:VAL:HG12	14	0.16
(1,634)	1:A:69:CYS:HB2	1:A:70:VAL:HG13	14	0.16
(1,607)	1:A:50:GLN:HB2	1:A:51:TYR:HA	1	0.16
(1,607)	1:A:50:GLN:HB2	1:A:51:TYR:HA	2	0.16
(1,607)	1:A:50:GLN:HB2	1:A:51:TYR:HA	14	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,607)	1:A:50:GLN:HB2	1:A:51:TYR:HA	17	0.16
(1,553)	1:A:24:LEU:HB3	1:A:26:THR:HA	8	0.16
(1,526)	1:A:16:ILE:HB	1:A:29:SER:HA	8	0.16
(1,514)	1:A:125:VAL:HB	1:B:205:PRO:HB2	1	0.16
(1,513)	1:A:5:PRO:HB2	1:B:325:VAL:HB	17	0.16
(1,433)	1:A:50:GLN:HG2	1:A:82:VAL:HG21	13	0.16
(1,433)	1:A:50:GLN:HG2	1:A:82:VAL:HG22	13	0.16
(1,433)	1:A:50:GLN:HG2	1:A:82:VAL:HG23	13	0.16
(1,433)	1:A:50:GLN:HG3	1:A:82:VAL:HG21	13	0.16
(1,433)	1:A:50:GLN:HG3	1:A:82:VAL:HG22	13	0.16
(1,433)	1:A:50:GLN:HG3	1:A:82:VAL:HG23	13	0.16
(1,306)	1:B:231:SER:HA	1:B:250:GLN:H	16	0.16
(1,200)	1:B:272:MET:H	1:B:273:PRO:HA	8	0.16
(1,199)	1:B:259:ALA:H	1:B:273:PRO:HA	19	0.16
(1,198)	1:A:72:MET:H	1:A:73:PRO:HA	7	0.16
(1,197)	1:A:59:ALA:H	1:A:73:PRO:HA	18	0.16
(1,163)	1:A:47:VAL:HG21	1:A:86:SER:HA	14	0.16
(1,163)	1:A:47:VAL:HG22	1:A:86:SER:HA	14	0.16
(1,163)	1:A:47:VAL:HG23	1:A:86:SER:HA	14	0.16
(1,154)	1:B:288:GLU:HB2	1:B:289:ASN:HA	9	0.16
(1,153)	1:A:88:GLU:HB2	1:A:89:ASN:HA	9	0.16
(1,1270)	1:B:315:LEU:H	1:B:317:PHE:H	20	0.16
(1,118)	1:B:293:LEU:HD11	1:B:294:LYS:HA	10	0.16
(1,118)	1:B:293:LEU:HD12	1:B:294:LYS:HA	10	0.16
(1,118)	1:B:293:LEU:HD13	1:B:294:LYS:HA	10	0.16
(1,1160)	1:B:250:GLN:H	1:B:250:GLN:HB2	20	0.16
(1,1142)	1:B:250:GLN:H	1:B:283:ILE:H	17	0.16
(1,97)	1:B:232:LEU:HD11	1:B:234:ARG:HA	5	0.15
(1,97)	1:B:232:LEU:HD12	1:B:234:ARG:HA	5	0.15
(1,97)	1:B:232:LEU:HD13	1:B:234:ARG:HA	5	0.15
(1,904)	1:B:303:ASN:H	1:B:325:VAL:HG21	9	0.15
(1,904)	1:B:303:ASN:H	1:B:325:VAL:HG22	9	0.15
(1,904)	1:B:303:ASN:H	1:B:325:VAL:HG23	9	0.15
(1,901)	1:A:103:ASN:H	1:A:125:VAL:HG21	9	0.15
(1,901)	1:A:103:ASN:H	1:A:125:VAL:HG22	9	0.15
(1,901)	1:A:103:ASN:H	1:A:125:VAL:HG23	9	0.15
(1,778)	1:A:32:LEU:HD11	1:B:316:GLY:H	14	0.15
(1,778)	1:A:32:LEU:HD12	1:B:316:GLY:H	14	0.15
(1,778)	1:A:32:LEU:HD13	1:B:316:GLY:H	14	0.15
(1,678)	1:A:93:LEU:HD11	1:A:94:LYS:HG2	12	0.15
(1,678)	1:A:93:LEU:HD12	1:A:94:LYS:HG2	12	0.15
(1,678)	1:A:93:LEU:HD13	1:A:94:LYS:HG2	12	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,658)	1:B:293:LEU:HD11	1:B:294:LYS:HG3	11	0.15
(1,658)	1:B:293:LEU:HD12	1:B:294:LYS:HG3	11	0.15
(1,658)	1:B:293:LEU:HD13	1:B:294:LYS:HG3	11	0.15
(1,657)	1:A:93:LEU:HD11	1:A:94:LYS:HG3	1	0.15
(1,657)	1:A:93:LEU:HD12	1:A:94:LYS:HG3	1	0.15
(1,657)	1:A:93:LEU:HD13	1:A:94:LYS:HG3	1	0.15
(1,657)	1:A:93:LEU:HD11	1:A:94:LYS:HG3	11	0.15
(1,657)	1:A:93:LEU:HD12	1:A:94:LYS:HG3	11	0.15
(1,657)	1:A:93:LEU:HD13	1:A:94:LYS:HG3	11	0.15
(1,648)	1:B:302:ARG:HG2	1:B:325:VAL:HA	16	0.15
(1,634)	1:A:69:CYS:HB2	1:A:70:VAL:HG11	1	0.15
(1,634)	1:A:69:CYS:HB2	1:A:70:VAL:HG12	1	0.15
(1,634)	1:A:69:CYS:HB2	1:A:70:VAL:HG13	1	0.15
(1,608)	1:B:250:GLN:HB2	1:B:251:TYR:HA	4	0.15
(1,608)	1:B:250:GLN:HB2	1:B:251:TYR:HA	11	0.15
(1,607)	1:A:50:GLN:HB2	1:A:51:TYR:HA	9	0.15
(1,607)	1:A:50:GLN:HB2	1:A:51:TYR:HA	16	0.15
(1,597)	1:B:249:GLY:H	1:B:250:GLN:HB2	13	0.15
(1,570)	1:B:259:ALA:HB1	1:B:272:MET:HB2	2	0.15
(1,570)	1:B:259:ALA:HB2	1:B:272:MET:HB2	2	0.15
(1,570)	1:B:259:ALA:HB3	1:B:272:MET:HB2	2	0.15
(1,553)	1:A:24:LEU:HB3	1:A:26:THR:HA	15	0.15
(1,449)	1:B:306:THR:HG21	1:B:322:ALA:HB1	20	0.15
(1,449)	1:B:306:THR:HG21	1:B:322:ALA:HB2	20	0.15
(1,449)	1:B:306:THR:HG21	1:B:322:ALA:HB3	20	0.15
(1,449)	1:B:306:THR:HG22	1:B:322:ALA:HB1	20	0.15
(1,449)	1:B:306:THR:HG22	1:B:322:ALA:HB2	20	0.15
(1,449)	1:B:306:THR:HG22	1:B:322:ALA:HB3	20	0.15
(1,449)	1:B:306:THR:HG23	1:B:322:ALA:HB1	20	0.15
(1,449)	1:B:306:THR:HG23	1:B:322:ALA:HB2	20	0.15
(1,449)	1:B:306:THR:HG23	1:B:322:ALA:HB3	20	0.15
(1,394)	1:B:324:ILE:HD11	1:B:325:VAL:HG21	1	0.15
(1,394)	1:B:324:ILE:HD11	1:B:325:VAL:HG22	1	0.15
(1,394)	1:B:324:ILE:HD11	1:B:325:VAL:HG23	1	0.15
(1,394)	1:B:324:ILE:HD12	1:B:325:VAL:HG21	1	0.15
(1,394)	1:B:324:ILE:HD12	1:B:325:VAL:HG22	1	0.15
(1,394)	1:B:324:ILE:HD12	1:B:325:VAL:HG23	1	0.15
(1,394)	1:B:324:ILE:HD13	1:B:325:VAL:HG21	1	0.15
(1,394)	1:B:324:ILE:HD13	1:B:325:VAL:HG22	1	0.15
(1,394)	1:B:324:ILE:HD13	1:B:325:VAL:HG23	1	0.15
(1,393)	1:A:124:ILE:HD11	1:A:125:VAL:HG21	16	0.15
(1,393)	1:A:124:ILE:HD11	1:A:125:VAL:HG22	16	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,393)	1:A:124:ILE:HD11	1:A:125:VAL:HG23	16	0.15
(1,393)	1:A:124:ILE:HD12	1:A:125:VAL:HG21	16	0.15
(1,393)	1:A:124:ILE:HD12	1:A:125:VAL:HG22	16	0.15
(1,393)	1:A:124:ILE:HD12	1:A:125:VAL:HG23	16	0.15
(1,393)	1:A:124:ILE:HD13	1:A:125:VAL:HG21	16	0.15
(1,393)	1:A:124:ILE:HD13	1:A:125:VAL:HG22	16	0.15
(1,393)	1:A:124:ILE:HD13	1:A:125:VAL:HG23	16	0.15
(1,375)	1:A:17:VAL:HB	1:A:27:THR:HB	20	0.15
(1,361)	1:B:216:ILE:HA	1:B:217:VAL:HG11	3	0.15
(1,361)	1:B:216:ILE:HA	1:B:217:VAL:HG12	3	0.15
(1,361)	1:B:216:ILE:HA	1:B:217:VAL:HG13	3	0.15
(1,359)	1:A:16:ILE:HA	1:A:17:VAL:HG11	15	0.15
(1,359)	1:A:16:ILE:HA	1:A:17:VAL:HG12	15	0.15
(1,359)	1:A:16:ILE:HA	1:A:17:VAL:HG13	15	0.15
(1,354)	1:B:217:VAL:HG11	1:B:218:TRP:HA	5	0.15
(1,354)	1:B:217:VAL:HG12	1:B:218:TRP:HA	5	0.15
(1,354)	1:B:217:VAL:HG13	1:B:218:TRP:HA	5	0.15
(1,354)	1:B:217:VAL:HG11	1:B:218:TRP:HA	19	0.15
(1,354)	1:B:217:VAL:HG12	1:B:218:TRP:HA	19	0.15
(1,354)	1:B:217:VAL:HG13	1:B:218:TRP:HA	19	0.15
(1,319)	1:B:275:GLU:HA	1:B:276:ASN:HB3	16	0.15
(1,200)	1:B:272:MET:H	1:B:273:PRO:HA	13	0.15
(1,159)	1:A:87:ALA:HA	1:A:90:LEU:HD21	4	0.15
(1,159)	1:A:87:ALA:HA	1:A:90:LEU:HD22	4	0.15
(1,159)	1:A:87:ALA:HA	1:A:90:LEU:HD23	4	0.15
(1,154)	1:B:288:GLU:HB2	1:B:289:ASN:HA	13	0.15
(1,1286)	1:B:233:LEU:H	1:B:249:GLY:H	12	0.15
(1,128)	1:B:293:LEU:HA	1:B:297:TRP:HA	15	0.15
(1,124)	1:B:293:LEU:HB2	1:B:294:LYS:HA	1	0.15
(1,1233)	1:A:17:VAL:HG11	1:A:28:PHE:H	18	0.15
(1,1233)	1:A:17:VAL:HG12	1:A:28:PHE:H	18	0.15
(1,1233)	1:A:17:VAL:HG13	1:A:28:PHE:H	18	0.15
(1,123)	1:A:93:LEU:HB2	1:A:94:LYS:HA	1	0.15
(1,123)	1:A:93:LEU:HB2	1:A:94:LYS:HA	17	0.15
(1,1223)	1:A:17:VAL:HG11	1:A:29:SER:H	7	0.15
(1,1223)	1:A:17:VAL:HG12	1:A:29:SER:H	7	0.15
(1,1223)	1:A:17:VAL:HG13	1:A:29:SER:H	7	0.15
(1,1219)	1:A:17:VAL:HA	1:A:30:ALA:H	11	0.15
(1,1194)	1:B:241:ILE:HB	1:B:242:ALA:H	10	0.15
(1,1161)	1:A:93:LEU:H	1:A:96:GLU:H	6	0.15
(1,112)	1:B:295:ALA:HA	1:B:298:GLU:HB3	1	0.15
(1,111)	1:A:95:ALA:HA	1:A:98:GLU:HB3	1	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,99)	1:A:94:LYS:HA	1:A:97:TRP:HA	13	0.14
(1,959)	1:A:92:THR:HG21	1:A:95:ALA:H	16	0.14
(1,959)	1:A:92:THR:HG22	1:A:95:ALA:H	16	0.14
(1,959)	1:A:92:THR:HG23	1:A:95:ALA:H	16	0.14
(1,921)	1:A:99:THR:HG21	1:A:101:LYS:H	19	0.14
(1,921)	1:A:99:THR:HG22	1:A:101:LYS:H	19	0.14
(1,921)	1:A:99:THR:HG23	1:A:101:LYS:H	19	0.14
(1,910)	1:A:103:ASN:H	1:A:124:ILE:HG21	20	0.14
(1,910)	1:A:103:ASN:H	1:A:124:ILE:HG22	20	0.14
(1,910)	1:A:103:ASN:H	1:A:124:ILE:HG23	20	0.14
(1,904)	1:B:303:ASN:H	1:B:325:VAL:HG21	18	0.14
(1,904)	1:B:303:ASN:H	1:B:325:VAL:HG22	18	0.14
(1,904)	1:B:303:ASN:H	1:B:325:VAL:HG23	18	0.14
(1,901)	1:A:103:ASN:H	1:A:125:VAL:HG21	18	0.14
(1,901)	1:A:103:ASN:H	1:A:125:VAL:HG22	18	0.14
(1,901)	1:A:103:ASN:H	1:A:125:VAL:HG23	18	0.14
(1,851)	1:A:97:TRP:HE1	1:B:305:ASP:H	13	0.14
(1,753)	1:A:106:THR:HG21	1:A:123:ALA:H	10	0.14
(1,753)	1:A:106:THR:HG22	1:A:123:ALA:H	10	0.14
(1,753)	1:A:106:THR:HG23	1:A:123:ALA:H	10	0.14
(1,753)	1:A:106:THR:HG21	1:A:123:ALA:H	11	0.14
(1,753)	1:A:106:THR:HG22	1:A:123:ALA:H	11	0.14
(1,753)	1:A:106:THR:HG23	1:A:123:ALA:H	11	0.14
(1,714)	1:A:103:ASN:HB2	1:A:125:VAL:H	2	0.14
(1,677)	1:A:90:LEU:HD11	1:A:94:LYS:HG2	8	0.14
(1,677)	1:A:90:LEU:HD12	1:A:94:LYS:HG2	8	0.14
(1,677)	1:A:90:LEU:HD13	1:A:94:LYS:HG2	8	0.14
(1,674)	1:B:287:ALA:HB1	1:B:288:GLU:HB3	13	0.14
(1,674)	1:B:287:ALA:HB2	1:B:288:GLU:HB3	13	0.14
(1,674)	1:B:287:ALA:HB3	1:B:288:GLU:HB3	13	0.14
(1,649)	1:A:114:GLY:HA3	1:A:115:LEU:HG	20	0.14
(1,608)	1:B:250:GLN:HB2	1:B:251:TYR:HA	5	0.14
(1,56)	1:B:303:ASN:HA	1:B:324:ILE:HA	10	0.14
(1,55)	1:A:103:ASN:HA	1:A:124:ILE:HA	4	0.14
(1,55)	1:A:103:ASN:HA	1:A:124:ILE:HA	10	0.14
(1,548)	1:A:69:CYS:HB3	1:A:70:VAL:HB	16	0.14
(1,503)	1:A:28:PHE:HA	1:A:54:VAL:HB	13	0.14
(1,434)	1:B:250:GLN:HG2	1:B:282:VAL:HG21	20	0.14
(1,434)	1:B:250:GLN:HG2	1:B:282:VAL:HG22	20	0.14
(1,434)	1:B:250:GLN:HG2	1:B:282:VAL:HG23	20	0.14
(1,434)	1:B:250:GLN:HG3	1:B:282:VAL:HG21	20	0.14
(1,434)	1:B:250:GLN:HG3	1:B:282:VAL:HG22	20	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,434)	1:B:250:GLN:HG3	1:B:282:VAL:HG23	20	0.14
(1,258)	1:A:28:PHE:HA	1:A:52:VAL:HB	3	0.14
(1,254)	1:B:217:VAL:HB	1:B:229:SER:HA	20	0.14
(1,200)	1:B:272:MET:H	1:B:273:PRO:HA	5	0.14
(1,197)	1:A:59:ALA:H	1:A:73:PRO:HA	2	0.14
(1,153)	1:A:88:GLU:HB2	1:A:89:ASN:HA	3	0.14
(1,1296)	1:A:97:TRP:HE1	1:B:305:ASP:HA	1	0.14
(1,1295)	1:A:105:ASP:HA	1:B:297:TRP:HE1	13	0.14
(1,1260)	1:B:314:GLY:H	1:B:315:LEU:HD21	2	0.14
(1,1260)	1:B:314:GLY:H	1:B:315:LEU:HD22	2	0.14
(1,1260)	1:B:314:GLY:H	1:B:315:LEU:HD23	2	0.14
(1,1260)	1:B:314:GLY:H	1:B:315:LEU:HD21	11	0.14
(1,1260)	1:B:314:GLY:H	1:B:315:LEU:HD22	11	0.14
(1,1260)	1:B:314:GLY:H	1:B:315:LEU:HD23	11	0.14
(1,1259)	1:A:114:GLY:H	1:A:115:LEU:HD21	2	0.14
(1,1259)	1:A:114:GLY:H	1:A:115:LEU:HD22	2	0.14
(1,1259)	1:A:114:GLY:H	1:A:115:LEU:HD23	2	0.14
(1,125)	1:A:93:LEU:HA	1:A:97:TRP:HA	13	0.14
(1,1234)	1:B:217:VAL:HG11	1:B:228:PHE:H	7	0.14
(1,1234)	1:B:217:VAL:HG12	1:B:228:PHE:H	7	0.14
(1,1234)	1:B:217:VAL:HG13	1:B:228:PHE:H	7	0.14
(1,1160)	1:B:250:GLN:H	1:B:250:GLN:HB2	13	0.14
(1,1078)	1:A:80:ARG:H	1:B:282:VAL:HG11	20	0.14
(1,1078)	1:A:80:ARG:H	1:B:282:VAL:HG12	20	0.14
(1,1078)	1:A:80:ARG:H	1:B:282:VAL:HG13	20	0.14
(1,974)	1:B:293:LEU:HD11	1:B:294:LYS:H	12	0.13
(1,974)	1:B:293:LEU:HD12	1:B:294:LYS:H	12	0.13
(1,974)	1:B:293:LEU:HD13	1:B:294:LYS:H	12	0.13
(1,95)	1:A:32:LEU:HD11	1:A:34:ARG:HA	5	0.13
(1,95)	1:A:32:LEU:HD12	1:A:34:ARG:HA	5	0.13
(1,95)	1:A:32:LEU:HD13	1:A:34:ARG:HA	5	0.13
(1,922)	1:B:299:THR:HG21	1:B:301:LYS:H	19	0.13
(1,922)	1:B:299:THR:HG22	1:B:301:LYS:H	19	0.13
(1,922)	1:B:299:THR:HG23	1:B:301:LYS:H	19	0.13
(1,851)	1:A:97:TRP:HE1	1:B:305:ASP:H	9	0.13
(1,754)	1:B:306:THR:HG21	1:B:323:ALA:H	10	0.13
(1,754)	1:B:306:THR:HG22	1:B:323:ALA:H	10	0.13
(1,754)	1:B:306:THR:HG23	1:B:323:ALA:H	10	0.13
(1,742)	1:B:324:ILE:H	1:B:324:ILE:HG12	11	0.13
(1,716)	1:B:303:ASN:HB2	1:B:325:VAL:H	5	0.13
(1,648)	1:B:302:ARG:HG2	1:B:325:VAL:HA	13	0.13
(1,608)	1:B:250:GLN:HB2	1:B:251:TYR:HA	9	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,607)	1:A:50:GLN:HB2	1:A:51:TYR:HA	20	0.13
(1,588)	1:B:222:THR:H	1:B:223:ARG:HD3	5	0.13
(1,586)	1:B:275:GLU:HG3	1:B:276:ASN:H	3	0.13
(1,507)	1:A:54:VAL:HB	1:A:78:SER:HA	20	0.13
(1,380)	1:B:227:THR:HB	1:B:254:VAL:HG21	20	0.13
(1,380)	1:B:227:THR:HB	1:B:254:VAL:HG22	20	0.13
(1,380)	1:B:227:THR:HB	1:B:254:VAL:HG23	20	0.13
(1,354)	1:B:217:VAL:HG11	1:B:218:TRP:HA	10	0.13
(1,354)	1:B:217:VAL:HG12	1:B:218:TRP:HA	10	0.13
(1,354)	1:B:217:VAL:HG13	1:B:218:TRP:HA	10	0.13
(1,354)	1:B:217:VAL:HG11	1:B:218:TRP:HA	13	0.13
(1,354)	1:B:217:VAL:HG12	1:B:218:TRP:HA	13	0.13
(1,354)	1:B:217:VAL:HG13	1:B:218:TRP:HA	13	0.13
(1,353)	1:A:17:VAL:HG11	1:A:18:TRP:HA	17	0.13
(1,353)	1:A:17:VAL:HG12	1:A:18:TRP:HA	17	0.13
(1,353)	1:A:17:VAL:HG13	1:A:18:TRP:HA	17	0.13
(1,318)	1:A:74:ASN:HB3	1:A:75:GLU:HA	18	0.13
(1,317)	1:A:75:GLU:HA	1:A:76:ASN:HB3	5	0.13
(1,31)	1:A:112:ASN:HA	1:A:115:LEU:H	13	0.13
(1,257)	1:A:17:VAL:HB	1:A:28:PHE:HA	2	0.13
(1,216)	1:B:251:TYR:HA	1:B:252:VAL:HB	12	0.13
(1,214)	1:A:51:TYR:HA	1:A:52:VAL:HB	3	0.13
(1,174)	1:B:248:SER:HA	1:B:283:ILE:HA	12	0.13
(1,16)	1:B:306:THR:HG21	1:B:322:ALA:HA	6	0.13
(1,16)	1:B:306:THR:HG22	1:B:322:ALA:HA	6	0.13
(1,16)	1:B:306:THR:HG23	1:B:322:ALA:HA	6	0.13
(1,159)	1:A:87:ALA:HA	1:A:90:LEU:HD21	17	0.13
(1,159)	1:A:87:ALA:HA	1:A:90:LEU:HD22	17	0.13
(1,159)	1:A:87:ALA:HA	1:A:90:LEU:HD23	17	0.13
(1,1295)	1:A:105:ASP:HA	1:B:297:TRP:HE1	14	0.13
(1,128)	1:B:293:LEU:HA	1:B:297:TRP:HA	10	0.13
(1,1269)	1:A:115:LEU:H	1:A:117:PHE:H	12	0.13
(1,125)	1:A:93:LEU:HA	1:A:97:TRP:HA	10	0.13
(1,1234)	1:B:217:VAL:HG11	1:B:228:PHE:H	8	0.13
(1,1234)	1:B:217:VAL:HG12	1:B:228:PHE:H	8	0.13
(1,1234)	1:B:217:VAL:HG13	1:B:228:PHE:H	8	0.13
(1,1219)	1:A:17:VAL:HA	1:A:30:ALA:H	1	0.13
(1,118)	1:B:293:LEU:HD11	1:B:294:LYS:HA	9	0.13
(1,118)	1:B:293:LEU:HD12	1:B:294:LYS:HA	9	0.13
(1,118)	1:B:293:LEU:HD13	1:B:294:LYS:HA	9	0.13
(1,117)	1:A:93:LEU:HD11	1:A:94:LYS:HA	15	0.13
(1,117)	1:A:93:LEU:HD12	1:A:94:LYS:HA	15	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,117)	1:A:93:LEU:HD13	1:A:94:LYS:HA	15	0.13
(1,112)	1:B:295:ALA:HA	1:B:298:GLU:HB3	17	0.13
(1,111)	1:A:95:ALA:HA	1:A:98:GLU:HB3	6	0.13
(1,1087)	1:B:278:SER:H	1:B:279:ILE:HG12	11	0.13
(1,1075)	1:A:82:VAL:HG11	1:B:280:ARG:H	13	0.13
(1,1075)	1:A:82:VAL:HG12	1:B:280:ARG:H	13	0.13
(1,1075)	1:A:82:VAL:HG13	1:B:280:ARG:H	13	0.13
(1,106)	1:B:295:ALA:HA	1:B:296:GLU:HG2	5	0.13
(1,106)	1:B:295:ALA:HA	1:B:296:GLU:HG3	5	0.13
(1,105)	1:A:95:ALA:HA	1:A:96:GLU:HG2	5	0.13
(1,105)	1:A:95:ALA:HA	1:A:96:GLU:HG3	5	0.13
(1,100)	1:B:294:LYS:HA	1:B:297:TRP:HA	15	0.13
(1,987)	1:A:89:ASN:HA	1:A:91:ALA:H	12	0.12
(1,973)	1:A:93:LEU:HD11	1:A:94:LYS:H	12	0.12
(1,973)	1:A:93:LEU:HD12	1:A:94:LYS:H	12	0.12
(1,973)	1:A:93:LEU:HD13	1:A:94:LYS:H	12	0.12
(1,919)	1:A:101:LYS:H	1:A:102:ARG:HB2	1	0.12
(1,919)	1:A:101:LYS:H	1:A:102:ARG:HB3	1	0.12
(1,910)	1:A:103:ASN:H	1:A:124:ILE:HG21	19	0.12
(1,910)	1:A:103:ASN:H	1:A:124:ILE:HG22	19	0.12
(1,910)	1:A:103:ASN:H	1:A:124:ILE:HG23	19	0.12
(1,904)	1:B:303:ASN:H	1:B:325:VAL:HG21	5	0.12
(1,904)	1:B:303:ASN:H	1:B:325:VAL:HG22	5	0.12
(1,904)	1:B:303:ASN:H	1:B:325:VAL:HG23	5	0.12
(1,901)	1:A:103:ASN:H	1:A:125:VAL:HG21	14	0.12
(1,901)	1:A:103:ASN:H	1:A:125:VAL:HG22	14	0.12
(1,901)	1:A:103:ASN:H	1:A:125:VAL:HG23	14	0.12
(1,798)	1:B:220:ASP:H	1:B:224:LEU:H	14	0.12
(1,754)	1:B:306:THR:HG21	1:B:323:ALA:H	19	0.12
(1,754)	1:B:306:THR:HG22	1:B:323:ALA:H	19	0.12
(1,754)	1:B:306:THR:HG23	1:B:323:ALA:H	19	0.12
(1,753)	1:A:106:THR:HG21	1:A:123:ALA:H	9	0.12
(1,753)	1:A:106:THR:HG22	1:A:123:ALA:H	9	0.12
(1,753)	1:A:106:THR:HG23	1:A:123:ALA:H	9	0.12
(1,753)	1:A:106:THR:HG21	1:A:123:ALA:H	14	0.12
(1,753)	1:A:106:THR:HG22	1:A:123:ALA:H	14	0.12
(1,753)	1:A:106:THR:HG23	1:A:123:ALA:H	14	0.12
(1,714)	1:A:103:ASN:HB2	1:A:125:VAL:H	18	0.12
(1,655)	1:A:93:LEU:H	1:A:94:LYS:HG2	10	0.12
(1,548)	1:A:69:CYS:HB3	1:A:70:VAL:HB	4	0.12
(1,526)	1:A:16:ILE:HB	1:A:29:SER:HA	12	0.12
(1,461)	1:A:103:ASN:HA	1:A:105:ASP:HB2	15	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,375)	1:A:17:VAL:HB	1:A:27:THR:HB	1	0.12
(1,353)	1:A:17:VAL:HG11	1:A:18:TRP:HA	1	0.12
(1,353)	1:A:17:VAL:HG12	1:A:18:TRP:HA	1	0.12
(1,353)	1:A:17:VAL:HG13	1:A:18:TRP:HA	1	0.12
(1,319)	1:B:275:GLU:HA	1:B:276:ASN:HB3	5	0.12
(1,174)	1:B:248:SER:HA	1:B:283:ILE:HA	18	0.12
(1,174)	1:B:248:SER:HA	1:B:283:ILE:HA	19	0.12
(1,153)	1:A:88:GLU:HB2	1:A:89:ASN:HA	15	0.12
(1,1287)	1:A:16:ILE:H	1:A:17:VAL:HA	17	0.12
(1,1270)	1:B:315:LEU:H	1:B:317:PHE:H	10	0.12
(1,1267)	1:A:17:VAL:HG11	1:A:19:SER:H	20	0.12
(1,1267)	1:A:17:VAL:HG12	1:A:19:SER:H	20	0.12
(1,1267)	1:A:17:VAL:HG13	1:A:19:SER:H	20	0.12
(1,1249)	1:A:70:VAL:HG11	1:A:72:MET:H	3	0.12
(1,1249)	1:A:70:VAL:HG12	1:A:72:MET:H	3	0.12
(1,1249)	1:A:70:VAL:HG13	1:A:72:MET:H	3	0.12
(1,1249)	1:A:70:VAL:HG11	1:A:72:MET:H	19	0.12
(1,1249)	1:A:70:VAL:HG12	1:A:72:MET:H	19	0.12
(1,1249)	1:A:70:VAL:HG13	1:A:72:MET:H	19	0.12
(1,1233)	1:A:17:VAL:HG11	1:A:28:PHE:H	14	0.12
(1,1233)	1:A:17:VAL:HG12	1:A:28:PHE:H	14	0.12
(1,1233)	1:A:17:VAL:HG13	1:A:28:PHE:H	14	0.12
(1,1225)	1:B:217:VAL:HG11	1:B:229:SER:H	4	0.12
(1,1225)	1:B:217:VAL:HG12	1:B:229:SER:H	4	0.12
(1,1225)	1:B:217:VAL:HG13	1:B:229:SER:H	4	0.12
(1,1194)	1:B:241:ILE:HB	1:B:242:ALA:H	13	0.12
(1,1162)	1:B:293:LEU:H	1:B:296:GLU:H	4	0.12
(1,1159)	1:A:50:GLN:H	1:A:50:GLN:HB2	13	0.12
(1,1155)	1:B:250:GLN:H	1:B:250:GLN:HG2	18	0.12
(1,1155)	1:B:250:GLN:H	1:B:250:GLN:HG3	18	0.12
(1,1153)	1:A:50:GLN:H	1:A:50:GLN:HG2	18	0.12
(1,1153)	1:A:50:GLN:H	1:A:50:GLN:HG3	18	0.12
(1,1142)	1:B:250:GLN:H	1:B:283:ILE:H	15	0.12
(1,1142)	1:B:250:GLN:H	1:B:283:ILE:H	18	0.12
(1,1078)	1:A:80:ARG:H	1:B:282:VAL:HG11	8	0.12
(1,1078)	1:A:80:ARG:H	1:B:282:VAL:HG12	8	0.12
(1,1078)	1:A:80:ARG:H	1:B:282:VAL:HG13	8	0.12
(1,1034)	1:A:79:ILE:HD11	1:B:284:SER:H	12	0.12
(1,1034)	1:A:79:ILE:HD12	1:B:284:SER:H	12	0.12
(1,1034)	1:A:79:ILE:HD13	1:B:284:SER:H	12	0.12
(1,1010)	1:B:286:SER:HA	1:B:288:GLU:H	18	0.12
(1,931)	1:B:232:LEU:HD11	1:B:233:LEU:H	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,931)	1:B:232:LEU:HD12	1:B:233:LEU:H	8	0.11
(1,931)	1:B:232:LEU:HD13	1:B:233:LEU:H	8	0.11
(1,912)	1:B:303:ASN:H	1:B:324:ILE:HG21	3	0.11
(1,912)	1:B:303:ASN:H	1:B:324:ILE:HG22	3	0.11
(1,912)	1:B:303:ASN:H	1:B:324:ILE:HG23	3	0.11
(1,905)	1:B:303:ASN:H	1:B:324:ILE:HG12	1	0.11
(1,904)	1:B:303:ASN:H	1:B:325:VAL:HG21	11	0.11
(1,904)	1:B:303:ASN:H	1:B:325:VAL:HG22	11	0.11
(1,904)	1:B:303:ASN:H	1:B:325:VAL:HG23	11	0.11
(1,902)	1:A:103:ASN:H	1:A:124:ILE:HG12	1	0.11
(1,897)	1:A:102:ARG:HG2	1:A:103:ASN:H	20	0.11
(1,754)	1:B:306:THR:HG21	1:B:323:ALA:H	9	0.11
(1,754)	1:B:306:THR:HG22	1:B:323:ALA:H	9	0.11
(1,754)	1:B:306:THR:HG23	1:B:323:ALA:H	9	0.11
(1,753)	1:A:106:THR:HG21	1:A:123:ALA:H	19	0.11
(1,753)	1:A:106:THR:HG22	1:A:123:ALA:H	19	0.11
(1,753)	1:A:106:THR:HG23	1:A:123:ALA:H	19	0.11
(1,722)	1:B:302:ARG:HB2	1:B:325:VAL:H	6	0.11
(1,722)	1:B:302:ARG:HB3	1:B:325:VAL:H	6	0.11
(1,690)	1:B:208:PRO:HG2	1:B:218:TRP:HB2	15	0.11
(1,690)	1:B:208:PRO:HG2	1:B:218:TRP:HB3	15	0.11
(1,690)	1:B:208:PRO:HG3	1:B:218:TRP:HB2	15	0.11
(1,690)	1:B:208:PRO:HG3	1:B:218:TRP:HB3	15	0.11
(1,674)	1:B:287:ALA:HB1	1:B:288:GLU:HB3	5	0.11
(1,674)	1:B:287:ALA:HB2	1:B:288:GLU:HB3	5	0.11
(1,674)	1:B:287:ALA:HB3	1:B:288:GLU:HB3	5	0.11
(1,673)	1:A:87:ALA:HB1	1:A:88:GLU:HB3	5	0.11
(1,673)	1:A:87:ALA:HB2	1:A:88:GLU:HB3	5	0.11
(1,673)	1:A:87:ALA:HB3	1:A:88:GLU:HB3	5	0.11
(1,673)	1:A:87:ALA:HB1	1:A:88:GLU:HB3	7	0.11
(1,673)	1:A:87:ALA:HB2	1:A:88:GLU:HB3	7	0.11
(1,673)	1:A:87:ALA:HB3	1:A:88:GLU:HB3	7	0.11
(1,673)	1:A:87:ALA:HB1	1:A:88:GLU:HB3	13	0.11
(1,673)	1:A:87:ALA:HB2	1:A:88:GLU:HB3	13	0.11
(1,673)	1:A:87:ALA:HB3	1:A:88:GLU:HB3	13	0.11
(1,656)	1:B:293:LEU:H	1:B:294:LYS:HG2	19	0.11
(1,648)	1:B:302:ARG:HG2	1:B:325:VAL:HA	6	0.11
(1,56)	1:B:303:ASN:HA	1:B:324:ILE:HA	13	0.11
(1,483)	1:A:119:ASP:HB3	1:A:120:PRO:HG2	13	0.11
(1,483)	1:A:119:ASP:HB3	1:A:120:PRO:HG3	13	0.11
(1,478)	1:B:308:PHE:HB2	1:B:310:SER:H	5	0.11
(1,477)	1:A:108:PHE:HB2	1:A:110:SER:H	19	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,438)	1:A:69:CYS:HA	1:A:70:VAL:HG11	19	0.11
(1,438)	1:A:69:CYS:HA	1:A:70:VAL:HG12	19	0.11
(1,438)	1:A:69:CYS:HA	1:A:70:VAL:HG13	19	0.11
(1,419)	1:B:307:LEU:HD11	1:B:322:ALA:HB1	20	0.11
(1,419)	1:B:307:LEU:HD11	1:B:322:ALA:HB2	20	0.11
(1,419)	1:B:307:LEU:HD11	1:B:322:ALA:HB3	20	0.11
(1,419)	1:B:307:LEU:HD12	1:B:322:ALA:HB1	20	0.11
(1,419)	1:B:307:LEU:HD12	1:B:322:ALA:HB2	20	0.11
(1,419)	1:B:307:LEU:HD12	1:B:322:ALA:HB3	20	0.11
(1,419)	1:B:307:LEU:HD13	1:B:322:ALA:HB1	20	0.11
(1,419)	1:B:307:LEU:HD13	1:B:322:ALA:HB2	20	0.11
(1,419)	1:B:307:LEU:HD13	1:B:322:ALA:HB3	20	0.11
(1,384)	1:B:227:THR:HB	1:B:254:VAL:H	14	0.11
(1,353)	1:A:17:VAL:HG11	1:A:18:TRP:HA	14	0.11
(1,353)	1:A:17:VAL:HG12	1:A:18:TRP:HA	14	0.11
(1,353)	1:A:17:VAL:HG13	1:A:18:TRP:HA	14	0.11
(1,352)	1:B:208:PRO:HA	1:B:218:TRP:HA	7	0.11
(1,32)	1:B:312:ASN:HA	1:B:315:LEU:H	13	0.11
(1,31)	1:A:112:ASN:HA	1:A:115:LEU:H	12	0.11
(1,294)	1:A:19:SER:HA	1:A:27:THR:HG21	8	0.11
(1,294)	1:A:19:SER:HA	1:A:27:THR:HG22	8	0.11
(1,294)	1:A:19:SER:HA	1:A:27:THR:HG23	8	0.11
(1,216)	1:B:251:TYR:HA	1:B:252:VAL:HB	6	0.11
(1,204)	1:B:265:CYS:HA	1:B:267:ASP:H	7	0.11
(1,199)	1:B:259:ALA:H	1:B:273:PRO:HA	5	0.11
(1,199)	1:B:259:ALA:H	1:B:273:PRO:HA	8	0.11
(1,197)	1:A:59:ALA:H	1:A:73:PRO:HA	3	0.11
(1,197)	1:A:59:ALA:H	1:A:73:PRO:HA	16	0.11
(1,148)	1:B:290:LEU:HB3	1:B:291:ALA:HA	11	0.11
(1,146)	1:A:90:LEU:HB3	1:A:91:ALA:HA	11	0.11
(1,1250)	1:B:270:VAL:HG11	1:B:272:MET:H	13	0.11
(1,1250)	1:B:270:VAL:HG12	1:B:272:MET:H	13	0.11
(1,1250)	1:B:270:VAL:HG13	1:B:272:MET:H	13	0.11
(1,125)	1:A:93:LEU:HA	1:A:97:TRP:HA	4	0.11
(1,1233)	1:A:17:VAL:HG11	1:A:28:PHE:H	9	0.11
(1,1233)	1:A:17:VAL:HG12	1:A:28:PHE:H	9	0.11
(1,1233)	1:A:17:VAL:HG13	1:A:28:PHE:H	9	0.11
(1,1216)	1:B:231:SER:H	1:B:252:VAL:HG11	6	0.11
(1,1216)	1:B:231:SER:H	1:B:252:VAL:HG12	6	0.11
(1,1216)	1:B:231:SER:H	1:B:252:VAL:HG13	6	0.11
(1,1162)	1:B:293:LEU:H	1:B:296:GLU:H	6	0.11
(1,1162)	1:B:293:LEU:H	1:B:296:GLU:H	13	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1141)	1:A:50:GLN:H	1:A:83:ILE:H	15	0.11
(1,1141)	1:A:50:GLN:H	1:A:83:ILE:H	18	0.11
(1,105)	1:A:95:ALA:HA	1:A:96:GLU:HG2	11	0.11
(1,105)	1:A:95:ALA:HA	1:A:96:GLU:HG3	11	0.11
(1,1034)	1:A:79:ILE:HD11	1:B:284:SER:H	15	0.11
(1,1034)	1:A:79:ILE:HD12	1:B:284:SER:H	15	0.11
(1,1034)	1:A:79:ILE:HD13	1:B:284:SER:H	15	0.11

10 Dihedral-angle violation analysis (i)

No dihedral-angle restraints found